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The MHOST Finite Element Program:
3-D Inelastic Analysis Methods for Hot Section Components
Volume I - Theoretical Manual

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16. Abstract This document discusses formulations and algorithms implemented in the MHOST finite element program developed under NASA Lewis Research Center Contract NAS3-23697. The code utilizes a novel concept of the <i>mixed iterative solution</i> technique for the efficient three dimensional computations of turbine engine hot section components. The second chapter is devoted to the general framework of variational formulations and solution algorithms derived from the mixed three-field <i>Hu-Washizu principle</i> . This formulation enables us to use nodal interpolation for coordinates, displacements, strains and stresses. Algorithmic description of the mixed iterative method includes variations for the quasi static, transient dynamic and buckling analyses. The global-local analysis procedure referred to as the <i>subelement refinement</i> is developed in the framework of the mixed iterative solution, of which the detail is presented also in the second chapter. The third chapter discusses the <i>numerically integrated isoparametric elements</i> implemented in this framework. Methods to filter certain components of strain and project the element discontinuous quantities to the nodes are developed for a family of linear elements. In the fourth section, we describe integration algorithms for linear and nonlinear equations included in the MHOST program. An appendix is added to outline the utilities handling the algebraic systems of linear equations such as the profile solver and subspace iterations for eigenvalue extraction.					
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SUMMARY

This document discusses formulations and algorithms implemented in the MHOST finite element program developed under NASA Lewis Research Center Contract NAS3-23697. The code utilizes a novel concept of the *mixed iterative solution* technique for the efficient three dimensional computations of turbine engine hot section components. We first survey the state-of-the-art finite element technology at the time when the project was started (1983) and the major contributions made by this effort in the advancement of the methodology since then. Also the formulations and methodologies developed under this project are summarized in the first introductory chapter. The second chapter is devoted to the general framework of variational formulations and solution algorithms derived from the mixed three-field *Hu-Washizu principle*. This formulation enables us to use nodal interpolation for coordinates, displacements, strains and stresses. Algorithmic description of the mixed iterative method includes variations for the quasi static, transient dynamic and buckling analyses. The global-local analysis procedure referred to as the *subelement refinement* is developed in the framework of the mixed iterative solution, of which the detail is presented also in the second chapter. The third chapter discusses the *numerically integrated isoparametric elements* implemented in this framework. Methods to filter certain components of strain and project the element discontinuous quantities to the nodes are developed for a family of linear elements. In the fourth section, we describe integration algorithms for linear and nonlinear finite element equations included in the MHOST program. An appendix is added to outline the utilities handling the algebraic systems of linear equations such as the profile solver and subspace iterations for eigenvalue extraction.

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1. INTRODUCTION

Introductory Remarks

The main objective of the MHOST finite element program development is to construct an efficient analysis package for three dimensional models of gas turbine engine hot section components incorporating various constitutive models describing the material response under extreme thermal and mechanical loading conditions. Another requirement was to represent quantities involved in the analysis at nodes. These are geometry (coordinates), deformation (displacement and deformation gradient), strain, stress and material parameters.

To fulfill the requirement, a new finite element formulation and solution algorithm is developed based on the mixed variational formulations. This concept enables us to introduce independent interpolation functions for all the physical quantities involved in the analysis, and to develop nodal interpolation algorithms. It was found from the literature survey that there had not been any formulation from which the efficient numerical procedure could be derived satisfying all the requirement stated in the first paragraph.

The most significant accomplishment in this finite element method development is that the *augmented Hu-Washizu principle* was constructed from which both element formulations and solution algorithms are derived. In the formulation and computer program developments for the MHOST system, other major ingredients are:

- (i) *The library of simple and efficient isoparametric elements;*
- (ii) *A set of nonlinear constitutive equations for modelling high temperature inelastic responses of hot section components;*
- (iii) *Efficient solution algorithms for quasi-static, dynamic and eigenvalue analysis;*
- (iv) *Friendly user interface in defining the finite element models and loading conditions; also for graphic post-processing and other applications such as the perturbation analysis for probabilistic structural analysis.*

The outline of this computational procedure differs radically from the conventional displacement method when applied to the linear elasticity. For nonlinear applications, the method works almost identical manner as the standard numerical

process. Indeed, one of the important findings in this project from the theoretical /numerical point of view is that the mixed iterative solution concept provides us with an rational framework to derive and analyze the solution strategies for nonlinear finite elements.

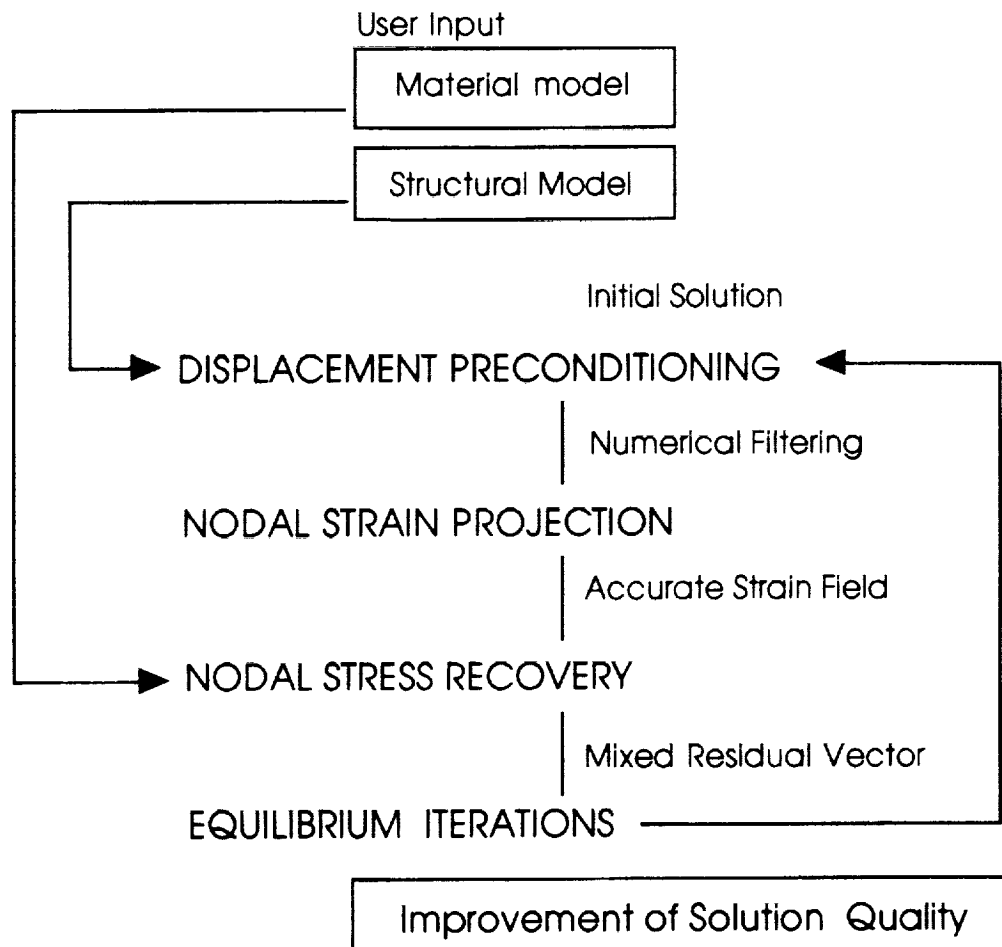


Figure 1.1 The Mixed Iterative Process. A Schematic Flow Chart.

Figure 1.1 illustrates the fundamental concept of mixed iterative solution strategy constructed directly from this mixed variational principle. The structural model is fed into the numerical computation in a usual way by constructing the displacement stiffness equations as the first step. Then the nodal strain is calculated by a mean square projection process, which eliminates the numerical instability in strain/stress approximations such as spurious oscillations. The inelastic material models are incorporated in the nodal stress integration in a modular fashion. The resulting nodally interpolated stress field is more accurate in comparison with the conventional displacement method. This improvement is brought back into the displacement finite element equations through the equilibrium iteration loop.

Additional computation required for the mixed iterative solution of linear problems is insignificant involving only a few re-solutions for the same stiffness matrix with modified residual vector. The nodal strain projection is carried out utilizing the diagonalized projection operator not requiring extra matrix manipulations. No additional computation is needed when the method is used for nonlinear computations. The modern iterative solution technology based on the quasi-Newton update is incorporated to further improve the performance of this solution method.

The system of finite element equations solved in the MHOST program is symbolically shown in Figure 1.2 with the equivalent mixed stiffness equations derived by the direct elimination. The construction and inversion of this mixed finite element equation is prohibitively expensive in terms of both the computing time and the memory requirement. Hence the iterative solution algorithms become attractive alternatives to overcome this difficulty and take advantages of the mixed finite element formulations.

Three Field Finite Element System

$$\begin{bmatrix} 0 & 0 & B \\ 0 & D & -C \\ B^t & -C^t & 0 \end{bmatrix} \begin{Bmatrix} U \\ E \\ S \end{Bmatrix} = \begin{Bmatrix} F \\ E_0 \\ 0 \end{Bmatrix}$$

Reduced Displacement Finite Element Equations

$$(B^t C^{-1} D C^t B) U = F - D E_0$$

Figure 1.2 The Mixed Finite Element Equations.

The linear convergence of the basic mixed iterative method is illustrated in Figure 1.3a. The difference of displacement and mixed stiffness matrices generates the driving residual vector for the iteration even for linear elastic problems. The quasi-Newton type update algorithms, with an example being illustrated in Figure 1.3b, improve the convergence rate of the iterative solution significantly.

In the MHOST program, other than the constant metric iteration scheme (somewhat similar to the modified Newton iteration) a family of modern iterative solution algorithms are implemented in order to improve the efficiency including; the optional line search, the conjugate gradient, the secant implementation of Davidon rank-one quasi-Newton, BFGS rank-two quasi-Newton update algorithms. We observe that the displacement stiffness gives steeper gradient in the load-deflection relation than the exact one, whereas the mixed stiffness lies in the flexible side. Therefore the

iterative solution algorithm starting from the displacement method gradually recovering the mixed solution is almost always stable and convergent.

To zoom-in to the local stress concentrations due to the embedded singularities such as holes and cracks, a scheme for global-local analysis referred to as *the sub-element* scheme is developed in the MHOST program. Elements requiring more detailed information in the global finite element computations are subdivided into a finer predefined mesh pattern, and the separate finite element computations are performed in these sub-element regions. The result is brought back to the global analysis by virtue of mixed iterative solution concept through the residual force vector generated by the sub-element stress field.

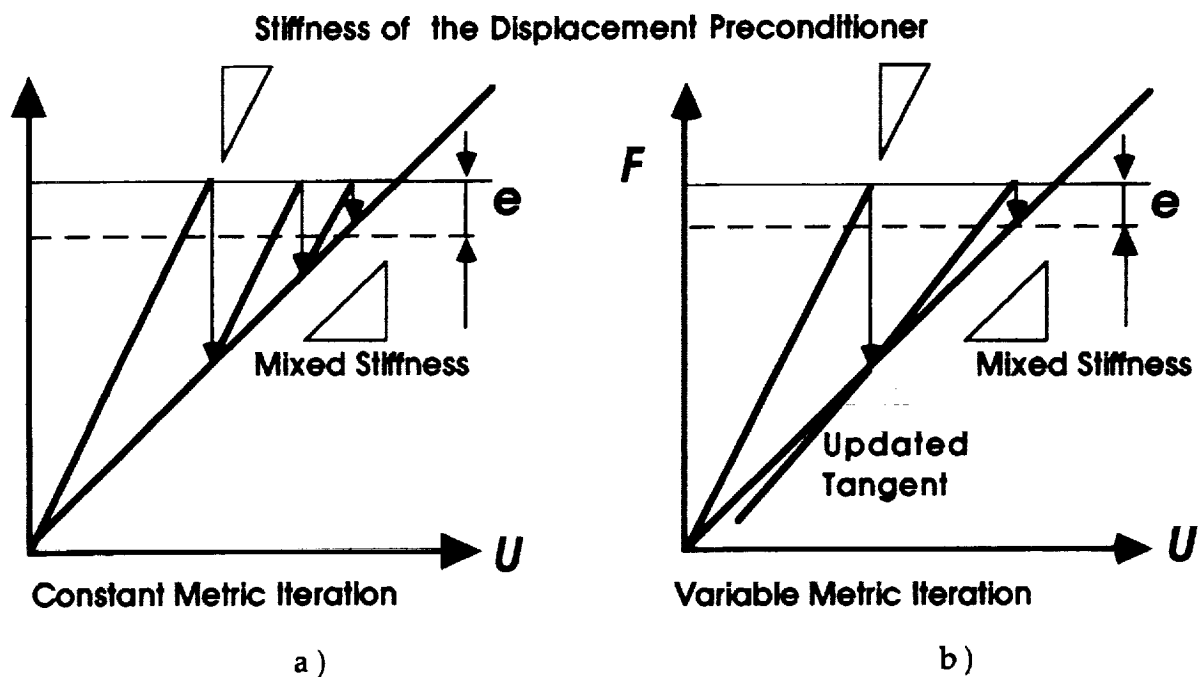


Figure 1.3 Behavior of the Mixed Iterative Solution. A Linear Problem.

The *numerically integrated isoparametric elements* are used in this work. To be able to increase the computing speed, only the linear basis functions are used for the global finite element computations. The element library consists of: *two node beam element* (type 98), *four node plane stress element* (type 3); *plane strain element* (type 11); *axisymmetric solid element* (type 10); *three dimensional solid element* (type 7); and, *shell element* (type 75). To be able to improve the accuracy, the selectively reduced integration scheme is incorporated with necessary refinements. Those are a rational *coordinate transformation and strain filtering mechanism* based on the polar decomposition of the isoparametric transformation and a *projection method* (often referred to as the *variational recovery method*) from the element discontinuous strain approximation to the nodal interpolation. A set of elements with high coarse mesh accuracy derived from the assumed stress concept (often referred to as the *assumed stress hybrid*

elements) is derived and included in the element library. Those are: plane stress (type 151), plane strain (type 152), axisymmetric solid (type 153), and three-dimensional solid (type 154).

The material models included in the MHOST program are:

- (i) *The linear elasticity with optional temperature dependency and anisotropy;*
- (ii) *The simplified plasticity (the secant elastic modulus is calculated in the stress recovery which is then used to generate the secant stiffness matrix representing the plastic response under the monotonic loading situations);*
- (iii) *The von Mises plasticity with the temperature dependent yield stress and the anisotropic yield surface definitions being the optional features. The radial return algorithm is used for the integration of the elastic-plastic material response over the given strain history. The general background of this type of algorithms is documented by HUGHES (1984). The finite deformation version of this algorithm implemented in this code is documented in NAGTEGAAL (1985). The effects of creep are taken into account in an explicit time integration algorithm constructed inside of the quasi-static solution subsystem.*
- (iv) *The unified viscoplastic constitutive equation originally developed by WALKER (1982) and implemented in a general purpose finite element package by CASSENTI (1983) is implemented in MHOST as a part of the material library. A straightforward explicit time integration with the substepping is used as the driving mechanism for the stress recovery. The temperature dependent isotropic elastic modulus is used as the preconditioner of the iterative solution incorporating this material model.*

The mechanism to incorporate other material models are provided in this computer program. As shown in Figure 1.1, the material definition is treated as another interface of the mixed iterative finite element method to the real world. The concept of *user subroutines* makes a wide range of different constitutive models easily implemented.

Historical Background

The research directions in the improvement of performance and applicability of the finite element method have continued to be:

- (i) *Mixed and hybrid formulations to improve the accuracy of the finite elements;*
- (ii) *Global solution procedures for linear and nonlinear finite element equations to reduce both the memory requirement and number of arithmetic operations with particular emphasis on the iterative solution strategies; and,*

- (iii) *Post-processing methods not only to accurately estimate errors a posteriori leading to adaptive mesh refinement strategies but also to extract more information out of a finite element solution.*

Equipped with the modern numerical technology and the advanced computing machinery, the application of finite elements expands its limit. The use of large meshes representing fine detail of the engineering problems has become useful. Sophisticated numerical methods have been developed to deal with combined nonlinear kinematics and material responses in a highly efficient manner.

Reports, books and journal articles related to the *non-standard* finite element methods are surveyed with the main objective being the search of useful numerical technology in the framework of mixed iterative solution algorithms. In the past, the *non-standard* finite element methods such as the mixed and hybrid method have not been exploited in a systematic manner. Few exceptions are the hybrid elements for plates and shell analysis which eventually generates the element *stiffness* equations and the mixed elements for incompressible problems based on the Lagrangian functional used by HERRMANN (1965).

As documented in TODD, CASSENTI, NAKAZAWA, BANERJEE (1984) and the research papers by NAKAZAWA (1984A,B), ZIENKIEWICZ, VILOTTE, NAKAZAWA, TOYOSHIMA (1984), ZIENKIEWICZ, LI, NAKAZAWA (1985), the iterative algorithms to develop continuous stress field such as developed by CANTIN, LOUBIGNAC, TOUZOT (1978) can be identified as the mixed finite element method. It is important to note that, in constructing the iterative methods, the use of Hu-Washizu variational principle is crucial to set up the practically useful algorithms, although a contrary remark is made in the classical textbook by ZIENKIEWICZ (1977) (page 310). In the recent paper by SIMO, TAYLOR, PISTER (1984), the same observation is made and a finite element method is constructed from the Hu-Washizu principle with application to the finite deformation plasticity.

Except for a few primitive papers such as mentioned above and the literature which appeared after the present development effort was initiated, no directly relevant work has been published on construction and iterative solution for the mixed finite element equation derived from the Hu-Washizu form. There are, however, a number of papers indirectly relevant to and somehow useful for the further development of solution strategy employed in the MHOST code.

The algorithm is viewed as composed of three steps. The linearized momentum equation is solved in terms of displacement vector for the pre-conditioning purposes. Then, the post-processing algorithm is entered to generate the strain field based on the mixed interpolation which is the used for the integration of the constitutive equation. The third step is the equilibrium iteration to satisfy the nonlinear virtual work equation with respect to the stress

field interpolated in a mixed manner.

The quality of displacement field generated by the preconditioning contributes significantly to the overall quality of the solution as well as the convergence characteristics. The use of equivalent stiffness to the element discontinuous strain mixed forms is a possible numerical strategy for these purposes [MALKUS, HUGHES (1978), HUGHES, MALKUS (1983)]. In particular, application to plates and shells in recent developments for the lower order element technology indicate possible improvements for the preconditioning operations [HUGHES, TEZDUYAR (1981)] with further efficiency gained by using the lower order quadrature [BELYTSCHKO, TSAY (1983)].

The strain recovery algorithm based on the mixed interpolation is found to be virtually identical to the classical methodology based on the consistent conjugate stress distribution studied by ODEN, BRAUCHLI (1971), ODEN, REDDY (1973). In the recent papers, BABUSKA, MILLER (1984) present a systematic method to construct and analyze the post-processing algorithms. It is claimed that there are postprocessing procedures for various quantities which have the same order of convergence rate as the energy error in the displacement finite element approximation. This statement agrees quite well with the experimental observation by OWA (1982), NAKAZAWA, OWA, ZIENKIEWICZ (1985). Also, the super convergent results in terms of stress and strain as well as the displacement observed in the first year exercise of this project may be due to the higher order convergence rate of the post-processing algorithm used for the strain recovery computation. No literature is available on the effect of numerical quadrature in the postprocessing algorithms except a recent technical note by SIMO, HUGHES (1985) on the assumed strain, so called B -bar type algorithms for continuum elements and plates and shells.

The integration algorithms of the nonlinear constitutive equations, in particular rate independent plasticity, are well- established as indicated in the Task I literature survey [FAHYRE, HUGHES (1983)] and one of the most reliable algorithm based on the radial return concept [NAGTEGAAL, DE JONG (1981)] is implemented. No systematic effort has yet been reported of the algorithm development for the advanced viscoplastic constitutive models including the temperature effect. Further literature search and original investigation is required in this field.

Methods of equilibrium iteration have been investigated in recent years and a number of useful papers and reports have appeared, some of which are mentioned in the previous literature survey report. A survey and series of experiment reported by ABDEL RAHMAN (1982) is found a useful collection of algorithms and numerical results with application to the nonlinear plates. Basic algorithms of Newton-Raphson and modified- and quasi-Newton methods are compared in the displacement method framework. As demonstrated later in this report, algorithms discussed in a classical report by MATTHIES, STRANG (1979) are found usable even in the content of the mixed iterative method.

The algorithms and convergence arguments directly applicable to the present

framework are only available from the literature on the augmented Lagrangian methods for the quadratic minimization problem with linear equality constraints such as incompressibility and the Dirichlet boundary condition. Possible improvement of the iterative procedure is indicated in FORTIN, GLOWINSKI (1982) and the numerical test examples studied by NAKAZAWA, VILOTTE, ZIENKIEWICZ (1984), ZIENKIEWICZ, VILOTTE, NAKAZAWA, TOYOSHIMA (1984) shows the significant improvement obtained by using such algorithms for the analysis of Stokes' flow. The mathematical discussions and algorithms are also found in GIRAULT, RAVIART (1979), TEMAM (1977). The original idea of the mixed iterative solution is, indeed, found in a historical work by ARROW, HURWICZ, UZAWA (1968) and the class of iterative algorithms for the mixed problems is referred to as the Uzawa method.

In the context of linear elastic finite element analysis, the use of mixed approximations and equilibrium iteration has appeared in an ad hoc fashion repeatedly in the history other than the work by CANTIN, et al. (1979). For nonconforming plate bending elements, CRISFIELD (1975) has proposed an iterative algorithm to improve the property of the numerical process. In the paper, the similarity of the concept based on a modified Hellinger-Reissner principle to the initial strain method iteration is pointed out. Also, an important observation is that all the significant changes occur in the first iteration of the mixed process of plates.

The implementation of mixed finite elements without iterative solution is the topic extensively studied several decades ago mainly with application to the linear problems in mechanics as discussed in a survey by ZIENKIEWICZ (1977). These experiences are found useful to avoid possible numerical difficulties particular in this methodology. This is an important issue to be investigated. The characteristics of the particular algorithm used as the post-processor needs to be understood in the mixed method framework so as to fulfill the necessary conditions for the stability and convergence. Regardless of the solution algorithm, the mixed method needs to satisfy the stability condition referred to as the Babuska-Brezzi condition in some sense [BABUSKA (1973), BREZZI (1974)]. However, when the equal order interpolations of displacement and stress are used, possible dissatisfaction of this condition is indicated by ODEN (1982). Possible oscillations of the numerical solution are indicated therein under special circumstances.

As experienced in the mixed/penalty finite element computations for incompressible problems, however, the implication of Babuska-Brezzi condition is not quite clear. As discussed by ZIENKIEWICZ, NAKAZAWA (1982), the stability can be achieved by using a class of unstable elements which violates the condition a priori but produces stable results incorporating a post-processing algorithm which satisfies the necessary condition for the stability

Modern development of the mixed finite element methods is mostly to set up the displacement stiffness matrix from the element discontinuous approximation for additional variables [TAYLOR, ZIENKIEWICZ (1982)]. The derivation of this class of methods is based on the equivalence theorem stated in MALKUS, HUGHES (1978). An

important development along this line is a generalization of the equivalence theorem proposed in ZIENKIEWICZ, NAKAZAWA (1984) indicating that for all the numerically integrated displacement finite element method, there exists an equivalent class of mixed methods based on the Hu-Washizu principle. This observation provides some insights to the iterative process with particular application to inelastic problems. As mentioned earlier, these developments of *reducible* mixed forms at the element level are useful mainly to construct the preconditioning system of equations as well as the fine tuning of the equilibrium iteration.

In developing high performance finite elements, the Hu-Washizu principle has become the most popular variational formulation from which numerical methods are derived. It seems the most natural approach, for instance, to derive algorithms for probabilistic structural analysis methods. Also, methods to evaluate elements based on mixed variational principles have been developed. In modern literature, the word *mixed* and *hybrid* finite elements are often used interchangeably and ambiguously. Seemingly, the mixed methods derived from piecewise discontinuous stress approximation are usually referred to as the hybrid formulations and those derived from independent strain interpolation and other mixed formulations are referred to as the mixed forms. It is interesting to note that the word *hybrid* is used by a certain sector of computational mechanics community referring to a class of methods combining the finite element and boundary integral formulations.

Attention has recently been paid to the equal order interpolation for the mixed finite element processes. Series of papers and reports have been coming out from not only this project but also the research group at Swansea. A number of academic research projects have been initiated in the recent few years.

The interest in the Hu-Washizu principle is rejuvenated by the untimely death of one of the original investigators and the publication of his memorial volume [PIAN (1984)]. Utilization of this principle for the analysis of existing methods such as numerically integrated displacement formulation [ZIENKIEWICZ, NAKAZAWA (1984)] appears in literature frequently. Belytschko (1986) reviews the technology available for the thick plate and shell element formulation based on the Reissner-Mindlin theory by this principle.

Efforts to use the mixed Hu-Washizu finite element equations as a driving mechanism for the iterative solution of linear and nonlinear problems are reported in recent publications [NAKAZAWA, NAGTEGAAL (1986), NAKAZAWA, SPIEGEL (1986)]. With particular application to transient dynamics, a version of the mixed iterative solution algorithm combined with a second order, single step time integration operator is proposed and applied to a number of linear elastic problems by ZIENKIEWICZ, LI, NAKAZAWA (1986).

An analysis of a certain class of mixed finite elements is discussed by LE TALLAC (1986). An iterative algorithm based on the Hu-Washizu principle is derived for rate-independent deviatoric plasticity. The elastic strain is used as a variable instead of the

total strain. This formal alteration of the formulation in conjunction with the radial return algorithm being hard-wired to the analysis enabled him to discuss the existence of solution which leads us to the possible formalization of convergence characteristics.

For the evaluation of element formulations and the first step of finite element code validation, the patch test invented by Irons and documented in BAZELEY, CHEUNG, IRONS, ZIENKIEWICZ (1956) has been used by many researchers and commercial code developers. NAGTEGAAL, NAKAZAWA, TATEISHI (1986) discuss the development of an eight-node shell element based on the assumed strain approach and demonstrate its validity by performing an extensive set of patch test.

The concept of patch test is re-examined in a recent paper by Taylor, Simo, ZIENKIEWICZ, CHAN (1986) where the equivalence between the satisfaction of the patch test and the consistency and stability of finite element approximations is discussed. Note that the argument by STUMMEL (1980) seriously questioning the validity of the patch test is countered in this paper.

An important extension of the patch test is proposed in a more recent paper by ZIENKIEWICZ, QU, TAYLOR, NAKAZAWA (1986). Assuming that the consistency of the approximations is satisfied, the test focuses upon the stability of mixed finite elements implied by the Babuska-Brezzi condition [BABUSKA (1973), BREZZI (1974)]. The procedure is to count the minimum possible number of active degrees-of-freedom in a patch and compare it with the maximum possible number of constraint degrees-of-freedom. If no constraints are imposed on nodal stresses and strains, the mixed, iterative solution procedure with continuous interpolation passes the test and is assumed stable. An extension of this stability patch test to three field formulations of Hu-Washizu type and for plates and shells derived from the Reissner-Mindlin theory is being investigated by ZIENKIEWICZ (1986) and his co-workers.

The relation between the stability patch test and the mathematically derived Babuska-Brezzi condition is also being actively investigated.

For the numerical modeling of singularities embedded in the structures, papers on the fracture mechanics are surveyed. For the displacement finite element technology, the report by FINE (1984) covers the technology to date. Except for a few academic exercises such as reported in ANNIGERI (1984), not many papers and research reports are available to mixed and hybrid finite elements with application to fracture mechanics, in particular, nonlinear material problems. A paper by BABUSKA, MILLER (1984) on the post-processing to detect the stress intensity factor is found useful to construct and validate the numerical algorithm to be implemented in the MHOST program. The general strategy for the numerical post-processing is extended to deal with problems with singularities.

A series of papers by BABUSKA et. al. (1984) discusses the possible utilization of the post-processing technology and the adaptive mesh refinement. The concept is closely related to the mixed iterative solution algorithms in conjunction with the

subelement calculation as discussed later in this report. Literature on the adaptivity and a posteriori (See GAGO (1982) and literature cited therein) error estimate is found useful in this line of development.

The methodology to compute the approximation error in a finite element solution has been improved significantly in the last few years. Also, the adaptive mesh refinement algorithms based on the spatial distribution of error indicator are developed and applied to a wide range of linear and nonlinear problems. A book on this subject is compiled by Gago which represents the state-of-the-art [BABUSKA, ZIENKIEWICZ, GAGO, OLIVERIA (1986)].

The papers included in the book indicate that a posterior error estimate and adaptive refinement methodologies are well understood mathematically and tested for a wide range of linear elastic problems. However, the computational processes look overly complicated and extensions to nonlinear analysis of solids and structures will need further research and development. Application of the adaptive mesh refinement concept has been demonstrated tractable using a relatively simple error indicator with application to aerospace flow problems given by the compressible Euler equations. Note that the adaptive solution of compressible Euler equations are the first systematic attempt of extending the technology to nonlinear problems. The results included in the book shows the potential advantage of the concept over the commonly used finite difference technology.

A simple algorithm to estimate error a posteriori is proposed by ZIENKIEWICZ, ZHU (1986). The logic is based on the difference of quantities obtained directly at the elements and the same information projected by nodal interpolation functions. The nodal projection techniques used in the mixed, iterative process to recover the nodal strain is the simple and effective way to calculate errors. This process is relatively simple to implement in comparison with seemingly complicated mathematically derived a posterior error estimate algorithms. Examples shown in the paper indicate the efficiency of the proposed process. However, rigorous mathematical analysis is still to be done to verify the methodology. It is interesting to note that the residual vector calculated in MHOST at the zeroth iteration of the equal order mixed iterative solution is indeed the Zienkiewicz-Zhu error indicator weight-averaged at nodes.

Using triangular elements, efforts to combine automatic mesh-generation and adaptive refinement concepts have been reported. Examples included in ZIENKIEWICZ, ZHU (1986) uses this idea. In application of adaptive mesh refinement to compressible flow problems, a number of papers are published in which triangular mesh generation methods were discussed with local refinement strategy to capture shocks. PERAIRE, MORGAN, ZIENKIEWICZ (1986), LOHNER (1986) discuss adaptive mesh refinement and de-refinement algorithm designed for the triangles and speculate the applicability of the concept to three-dimensional computations. The use of automatic mesh generation of triangular and tetrahedral elements has been found a useful trick in finite difference flow computations using unstructured grid. JAMESON (1986) demonstrated possible utilization of this technology for geometrically complex

problems.

In the area of a posteriori error estimates, post-processing and adaptive mesh refinement, useful technology has been developed for linear structural analysis and certain nonlinear problems. However, further research and development including extensive numerical experiments are required to establish a methodology usable for three-dimensional inelastic analyses involving complex loading histories.

A series of note by AXELSSON (1976, 1978) indicates the possible utilization of successive relaxation techniques for the solution of finite element equations, in particular, the mixed system of equations. However, no evidence that such algorithms can be used for nonlinear solution is provided in those publications.

Application of finite element methods to nonlinear structural analysis involves increasingly complicated geometrical and material models and utilizes performance of currently available supercomputing facilities to their limits. Codes specifically designed for supercomputers have demonstrated their potential. Papers have appeared recently discussing performance improvement of finite element codes on vector and parallel machines utilizing algorithms tailored for specific computer environment. BENSON, HALLQUIST (1986) discusses the rigid body algorithm implemented in DYNA code which reduced the amount of computations significantly in explicit finite element time integrations. Implementation of an iterative solution algorithm based on the element-by-element preconditioner in NIKE code is discussed by HUGHES, FERENCZ, HALLQUIST (1986). The utilization of supercomputers in an engineering environment involving the development of these codes is presented by GOUDREAU, BENSON, HALLQUIST, KAY, ROSINSKY, SACKETT (1986).

Investigations of vectorizability of basic finite element operations continue. For instance, the detail of vector-matrix multiply in element-by-element manner is discussed including timing figures for various finite element models by HAYES, DEVLOO (1986). An algorithm to potentially take full advantage of vector machines to solve a system of ordinary differential equations is proposed by Brown, Hindmarsh (1986). Iterative algorithms based on the ORTHOMIN method and incomplete factorization are studied by ZYVOLOSKI (1986). It is anticipated that the development of algorithms closely tied to the actual data manipulations and arithmetic operations in computing machineries will eventually lead us to write faster finite element codes not only on supercomputers but also on smaller scalar machines.

Utilization of parallel computing for the equation solution is a subject investigated extensively in the last few years. A series of papers by Utku, Melosh and their collaborators look into the possible parallelization of direct stiffness matrix factorization [UTKU, MELOSH, SALAMA, CHANG (1986), UTKU, SALAMA, MELOSH (1986)]. The possible utilization of hypercube architecture is studied by NOUR-OMID, ORTIZ (1986) for the factorization and iterative solution of finite element equations. It is observed in these papers that the plain reduction of total number of operation does not always provide an optimal algorithm for vector and parallel processing. Increasing number of sessions are devoted to discuss this aspect of finite element computations in

scientific meetings, and literature is being accumulated. However, further research and development still needs to be done before robust algorithms become available for a wide range of engineering applications which fully utilize the potential of modern computing machineries.

Notable progress has been made in the last few years in the field of computational plasticity, in particular, design and analysis of integration algorithms for rate-independent plasticity constitutive equations. ORTIZ, SIMO (1986) summarizes the development of integration algorithms and investigates the accuracy in great detail. The basic idea is to generalize the return mapping algorithm based on the elastic predictor. An extension to viscoplastic constitutive equations are included in this paper. SIMO (1986) extends the results to finite deformation plasticity developing a simple and efficient finite element algorithm in which elastic deformation of finite amplitude is accommodated.

Approaches to capture the localization due to the inelastic material response in global finite element computation have been developed which enable one to capture discontinuities occurring at subelement scale. The work by HUGHES, SHAKIB (1986) extends the conventional return mapping algorithm for J_2 -flow theory to the yield surfaces with corners. This extension can be used to capture the effects of localized plastic flow in a global manner. ORTIZ, LEROY (1986) proposes an algorithm which allows shear bands to generate inside of a finite element. The numerical results indicate the potential of the method to capture local failure of structures without excessive mesh refinement. Ideas to bring in the local failure mode in finite elements to capture localization effects under strain softening are discussed by WILLAM, SOBH, STURE (1986). A survey of the finite element technology for capturing the localized failure modes is given by NEEDLEMAN (1986). This is a relatively new field and further work will lead us to effectively calculate the localized microscopic material responses due to the embedded singularities in large scale structural systems.

In the theoretical aspects of finite element development, the utilization of mixed variational principle has been and will be the main thrust of the research and development. This approach not only provides us with tools to improve the performance of elements but also lets us get a deep insight on the solution algorithms for linear and nonlinear problems. The mixed iterative methodology developed under HOST contract takes full advantage of these modern theoretical developments. Also, new ideas demonstrated in the MHOST program has attracted academic research interest in the computational mechanics community.

In the application and computational aspects of finite elements, significant progress made in the last few years has not been fully incorporated in the MHOST computer code development. The information available in literature indicates that further development to utilize modern algorithms and coding technology would enhance the performance of the MHOST code considerably.

2. VARIATIONAL FORMULATION AND COMPUTATIONAL PROCEDURES

Introductory Remarks

This chapter is devoted to the problem statement and its solution strategy of a class of problems dealt with in the framework of MHOST finite element program package. We first establish the notation used throughout this report in the form of the differential equations and then derive the variational statement suitable for the construction of the mixed iterative finite element analysis. In order to maintain the generality, the nonlinear transient problems used as the vehicle for this development in which the conventional quasi-static problems are included as a subclass.

The Global Solution Strategy

The nonlinear problem to describe the inelastic response of a material body in an open, bounded domain Ω with sufficiently smooth boundary $\partial\Omega$ is stated in this section and an augmented form of the generalized nonlinear Hu-Washizu variational principle is derived in the infinitesimal deformation setting. A generic solution algorithm is constructed which is valid for the quasi-static and the dynamic-transient analysis.

The procedure discussed here can be incorporated with various solution algorithms and time integration operators other than the conventional Newton-Raphson and Newmark- β methods.

The equilibrium equation is written in terms of Cartesian components of stress tensor as:

$$-\sigma_{ij,i} = \rho(f_j - a_j) \quad \text{in} \quad \Omega \quad (2.1)$$

where ρ is the material density, assumed constant, with σ , a and f being the stress tensor, the acceleration vector and the body force vector, respectively.

We assume a rate constitutive equation in a generic form

$$\dot{\sigma}_{ij} = D_{ijkl} \dot{\epsilon}_{kl} \quad (2.2)$$

with D and ε being the material modulus and strain tensor respectively. The strain components are given by

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) + \varepsilon_{ij}^0 \quad (2.3)$$

with ε^0 being the initial strain due to the thermal expansion and creep effects. Usual equality constraints for the displacement components are imposed on the boundary such that

$$u_j = \bar{u}_j \quad \text{on } \partial\Omega_1 \quad (2.4)$$

and

$$t_j = \sigma_{ij} n_i = t_j^0 \quad \text{on } \partial\Omega_2 \quad (2.5)$$

The weak variational form associated with the above problem statement is

$$(\sigma_{ij}, u_{i,j}^*) = (\rho(f_j - a_j), u_j^*) + \langle t_j^0, u_j^* \rangle \quad (2.6)$$

$$(\varepsilon_{ij}^*, [\sigma_{ij} - D_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^0)]) = 0 \quad (2.7)$$

and

$$(\sigma_{ij}^*, [\varepsilon_{ij} - \frac{1}{2}(u_{i,j} + u_{j,i})]) = 0 \quad (2.8)$$

where (\cdot, \cdot) denotes the usual L_2 inner product over the domain, defined by

$$(u, v) = \int_{\Omega} u v \, dx \quad u, v \in L_2(\Omega)$$

and $\langle \cdot, \cdot \rangle$ is the integral defined on the boundary defined by

$$\langle u, v \rangle = \int_{\partial\Omega} u v \, dx \quad u, v \in L_2(\partial\Omega)$$

with the superscript $*$ indicating the arbitrary variations from an appropriate space of admissible functions.

Elimination of the stress and the strain from the above system of variational equations results in the virtual work equation in terms of displacement

$$a(u, u^*) - (f, u^*) = 0 \quad (2.9)$$

with $a(.,.)$ being the usual energy product defined by

$$a(u, v) = \int_{\Omega} u_{i,j} D_{ijkl} v_{j,i} dx$$

The essential boundary condition, Equation (2.5) can be incorporated by virtue of penalty

$$a(u, u^*) + \varepsilon^{-1} \langle u - u^0, u^* \rangle = 0 \quad (2.10)$$

or equivalently

$$\begin{aligned} & (\sigma_{ij}, u_{i,j}^*) + \varepsilon^{-1} \langle u - u^0, u^* \rangle \\ & = (\rho(f_j - a_j), u_j^*) + \langle t_j^0, u_j^* \rangle \end{aligned} \quad (2.11)$$

It is obvious that the simultaneous weak variational statements, Equation (2.6 - 2.8), can be derived directly from the Hu-Washizu principle. This observation implies that the boundary conditions, Equations (2.4) and (2.5), are entered to the system of equations only via the conservation law for the linear momentum. In this setting imposition of boundary conditions for stress and strain is unnecessary. If such conditions are applied, the well-posedness of the problem may be disturbed yielding erroneous solution or possibly a rank deficient system of equations.

Note that the penalization for the Dirichlet boundary condition does not require the space of admissible variation to fulfill the homogeneous counterpart of the same condition.

Using the equal order interpolation function for all the variables involved in the analysis, we have

$$u_j^h = N_K U_{jK} \quad (2.12A)$$

$$a_j^h = N_K a_{jK} = N_K \ddot{u}_{jK} \quad (2.12B)$$

$$\varepsilon_{ij}^h = N_K E_{ijK} \quad (2.12C)$$

$$\sigma_{ij}^h = N_K S_{ijK} \quad (2.12D)$$

and for the data

$$f_j^h = N_K F_{jK} \quad (2.12E)$$

$$\varepsilon_{ij}^{0h} = N_K E_{ijK}^0 \quad (2.12F)$$

resulting in a system of algebraic equations

$$\begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{B} \\ \mathbf{0} & \mathbf{D} & -\mathbf{C} \\ \mathbf{B} & -\mathbf{C}^t & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{U} \\ \mathbf{E} \\ \mathbf{S} \end{Bmatrix} = \begin{Bmatrix} \mathbf{F} - \mathbf{MA} \\ \mathbf{G} \\ \mathbf{0} \end{Bmatrix} \quad (2.13)$$

where the submatrices are defined as

$$\mathbf{U} = \{U_{iL}\} \quad \mathbf{E} = \{E_{jkL}\} \quad \mathbf{S} = \{S_{jKL}\}$$

$$\mathbf{B} = [B_{ijkKL}] \quad B_{ijkKL} = \int_{\Omega} N_{K,j} N_L dx$$

$$\mathbf{C} = [C_{ijklKL}] \quad C_{ijklKL} = \int_{\Omega} N_K N_L dx$$

$$\mathbf{D} = [D_{ijklKL}] \quad D_{ijklKL} = \int_{\Omega} N_K E_{ijkl} N_L dx$$

$$\mathbf{M} = [M_{ijKL}] \quad M_{ijKL} = \rho \int_{\Omega} N_K N_L dx$$

with the loading vectors defined by

$$\mathbf{F} = [F_{iL}] \quad F_{iL} = \int_{\Omega} N_L \rho f_i dx + \int_{\partial\Omega} N_L \hat{t}_i ds$$

$$\mathbf{G} = [G_{ijL}] \quad G_{ijL} = \int_{\Omega} N_L E_{ijkl} \varepsilon_{kl}^0 dx$$

Note here, for the sake of simplicity, the integrated form of the rate constitutive

equation is assumed. We shall discuss the detail of incremental process and the stress recovery later in this chapter. The elimination of the nodal strain and stress lead to a *displacement solution* form:

$$\{ (B(C)^{-t} D(C)^{-1} B^t) + P \} U = \hat{F} - Ma \quad (2.14)$$

with

$$\hat{F} = F + \{ B(C)^{-t} D(C)^{-1} G \} \quad (2.15)$$

whereas the standard finite element form based on the statement (2.9) is approximated by a somewhat simpler form

$$(K + P)U = \hat{F} - Ma \quad (2.16)$$

An iterative solution algorithm is constructed first to the quasi-static counterpart of Equation (2.13) assuming the time derivatives of displacement vector are sufficiently small:

- (i) Initialize the residual and displacement vector

$$R := 0 ; U := 0$$

- (ii) Solve the preconditioning equations to update the displacement such that

$$U := U + A^{-1}(\hat{F} - R) \quad (2.17)$$

- (iii) Recover the nodal strain

$$E := C^{-1} B U - E^0 \quad (2.18)$$

- (iv) Integrate the constitutive equation

$$S := \int_{\tau} D(S, E) E d\tau \quad (2.19)$$

with t being the quasi-time associated with deformation history.

- (v) Evaluate the residual

$$R := \hat{F} - B S \quad (2.20)$$

- (vi) If the residual is small enough then exit; or else repeat from the step (ii).

As is obvious from the above discussion, the choice of the preconditioner A is crucial to obtain the convergence characteristics necessary for the practical implementations. For instance, if we can construct

$$A = \{ (B(C)^{-t} D(C)^{-1} B') + P \} \quad (2.21)$$

then no iteration is needed. However, the sparseness of the finite element system of matrix is no longer exploited if the above form were to be utilized. As a reasonable compromise, we use the augmented equilibrium equation by the displacement stiffness matrix which is to set

$$A = K + P \quad (2.22)$$

Other methods of preconditioning has been investigated but so far no robust scheme is known for a wide range of solid and structural analysis. See for instance, MULLER, HUGHES (1984). Except for minor modifications, the present solution utilizes the form defined by Equation (2.22).

Global-Local Analysis by Subelement Iterations

Computational fracture mechanics aspects are discussed in this note of the inelastic analysis of turbine engine hot section components. The motivation of this endeavor is to seek an economically feasible numerical process without sacrificing the accuracy of the solution.

The standard finite element method is to take the effect of embedded singularities into account by refining the mesh subdivision in the neighborhood of such points or alternatively to introduce special elements with singular functions in the same region. This currently available approach is often prohibitively expensive especially when it is applied to the analysis of a structure with multiple singularities of which each needs special treatment.

The use of nonstandard schemes, in particular the mixed finite element form, is found in the previous section far more advantageous compared with the conventional schemes with application to regular nonlinear structural analysis. Hence its utilization for the problems including singularities is worth investigating to realize a major breakthrough in the computational fracture mechanics.

The main objective to use the mixed finite element method for problems with embedded singularities is that higher resolution for stresses and strains is to be obtained without excessive mesh refinement for the displacement variables near

the singularities.

In the framework of displacement finite element method, only available information primarily from the computation is the nodal displacements from which the strain/stress components are calculated by differentiating the shape functions. Then these quantities are used to evaluate the fracture mechanics related quantities such as the stress concentration factor and the J- integrals.

Noting that the accuracy of strain/stress components is a full one order less than that of displacement for the displacement finite element method even without a singularity. Moreover, the approximation of strains/stresses could be extremely unstable near singularities and the area where the deformation is highly concentrated. To obtain accurate results for a problem with embedded singularities by the displacement technology, the mesh refinement at around the singularities is unavoidable so as to obtain accurate and stable displacement field which indeed is the only source to generate the strain/stress approximations. For the best possible results, monitoring a posteriori error indicator and several passes of (adaptive) mesh refinement are advisable for such calculations.

When the strains or stresses, sometimes both, are included explicitly in the finite element system of equations, in particular interpolated by C^0 - continuous basis functions, the resulting approximations are not only accurate but also stable having no spurious modes in the strain/stress recovery operator.

For regular problems, the numerical representation of stress field in particular is quantitatively accurate due to the equilibrium condition being explicitly evaluated by the approximate stress field itself. Compared with the displacement method, a full one order improvement is indeed expected of the convergence rate for the mixed method for the same mesh subdivision. It is noticed that the role of displacement solution in the mixed form is to generate qualitatively the deformation mode from which indirectly the deformation gradient is extracted and fed into the stress recovery and equilibrium iteration operations. Therefore the quantitative measure for error in displacement vector contributes relatively less significantly to the overall evaluation of fracture related quantities.

The approximate solution procedure for a deformable body with embedded singularities is first to solve the structural problem without crack which shall be specifically referred to as the global system and then to compute the deformation and the stresses near the singularity separately. This portion of the domain is called the local system. The concept is somewhat similar to the substructuring in the conventional finite element computations.

Topologically the global mesh is constructed such that the minimum element

size is much larger than the scale of singularities so that no singularity is identified by the global system. The local system is constructed in a single global element and coupled with the global system through common nodes between the global and local elements within.

A major difference of the present approach from the substructuring is that the local refinement takes place a posteriori and the information extracted from the locally subdivided element is brought back to the global mesh via the residual load correction. This implies that no special algebraic treatment is required even when the material nonlinearity occur in the sub-element region.

The solution strategy is indeed a mixed version of the hierarchic finite element process which has been investigated in the recent few years and the results obtained are encouraging for elastic stress analyses with singularities. The computational strategy we propose here is to define the local mesh and the refined interpolation altogether in the region near the singularity somewhat similar to combined h - p refinement.

As the result, we shall obtain accurate stress-strain solution in the global approximation subspace enriched by the local approximations.

The final solution to be obtained is in the global-local system with the global system being used only for preconditioning purposes. This means that the factorization of approximate global stiffness matrix obtained by the conventional displacement method may be sufficient to kick off the present solution procedure.

Consider as the second example a single displacement element with an embedded singularity, a hole. Some computational aspects need to be considered here with application of present method to practical problems of turbine engine hot section components. From the programming point of view, a parametric representation of an elliptic hole by its size, orientation and location in a displacement element is convenient allowing the code to generate subelement mesh data whenever this calculation is performed. The data structure could be simple as no permanent storage allocation is required for the subelement mesh. In Figure 2.1, an example of such a ready made subelement mesh is presented for a circular hole located at the center of displacement element mesh.

On the other hand, it may be user friendly and perhaps conceptually more general to explicitly define the subelement mesh as an additional data set. The data structure then needs to be reviewed so as to allocate additional memory for subelement mesh storage.

As experienced in the h -version of adaptive mesh refinement, it is anticipated that the concept of subelement mesh could be used recursively in a similar

fashion as the multi-level substructure technique. A well organized data storage scheme needs to be developed to realize the fully flexible implementation of the proposed scheme. In the following discussions, the subelement mesh is defined in the isoparametric element coordinate system rather than the physical space in which the global mesh is defined.

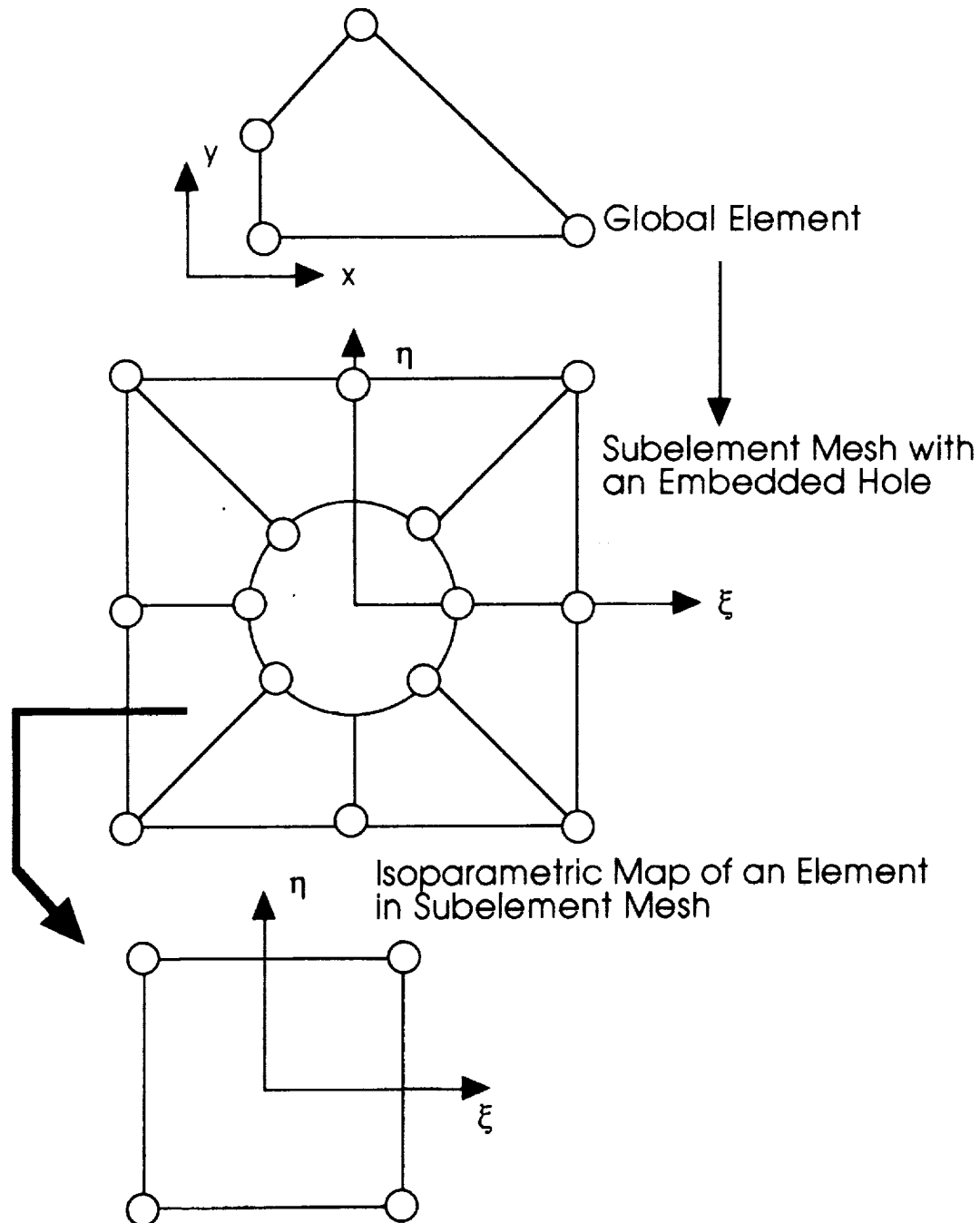


Figure 2.1 Multiple Mapping in the Subelement Mesh Refinement

The stresses and strains are represented at the nodes of subelement defined in the first reference plane in an exactly same manner as the one dimensional example.

We introduce variables to characterize the internal deformation of stress and strain subelement so as to obtain these quantity uniquely in an accurate manner. As mentioned in the first section, some further mathematical investigation is required to come up with an optimal combination of subelement mesh definition, functions to represent the deformation of subelement and the stress-strain interpolations.

A major difficulty encountered in the multidimensional computation is to integrate the coupling matrix B over the subelement. Noting that once the size of hole and its location are identified, the values of displacement interpolation functions are obtainable at every nodal point of subelements. Denoting these quantities by N, we introduce the local displacement-type interpolation of N in these elements by

$$N = N_K^S N_K \quad (2.23)$$

and the coupling matrix is integrated approximately by

$$B^S = \left[\int_S \frac{\partial N_K^S}{\partial(\xi, \eta)} N_L^S d\xi d\eta N_K \right] \quad (2.24)$$

where the superscript S denotes the functions defined at the subelement level. The calculation is carried out on each local subelement Ω^S and summed over the global displacement element. This general integration procedure plays a central role to couple the global and local mesh representing the residual load vector at the global displacement node entries yet reflecting the information at the local element level. For the consistent definition of this operator matrix, the transformation of shape function from global to local needs to be carried out as defined by Equation (2.23) on the isoparametric element space which is again mapped into another isoparametric space defined on each subelement. It is obvious that the location of nodal points needs to be given in the element coordinate system.

When the location of subelement nodal points are specified in the physical plane, the inverse of nonlinear isoparametric mapping needs to be calculated to locate them in the element coordinate system.

We outline the solution strategy in a general format. First we introduce the conventional stiffness equation with respect to the local hierarchial displacement

degree of freedom U as the preconditioner, which is

$$K^S U^S = F^S; \quad F^S = F^G - B^S S^G \quad (2.25)$$

derived directly from the virtual work principle in terms of displacement. A modified recursive form of mixed finite element equations is written again in terms of local unknown variables

$$\begin{bmatrix} K^S & 0 & B^S \\ 0 & D & -C^S \\ B^{St} & -C^{St} & 0 \end{bmatrix} \begin{Bmatrix} U^S \\ E^S \\ S^S \end{Bmatrix} = \begin{Bmatrix} F^S + K^S U^S \\ 0 \\ 0 \end{Bmatrix} \quad (2.26)$$

Setting $U^{(0)} = 0$ and $S^{(0)} = 0$ with the superscript being used for the iteration counter, we solve the system of displacement equation

$$U^{(n+1)S} = U^{(n)S} + (K^S)^{-1} \{ F^S - B^S S^{(n)S} \} \quad (2.27)$$

Then the stresses and strains are updated in the subelement region by solving iteratively with u being the enriched displacement in the subelement region. To obtain this quantity, the factorization of displacement type stiffness equation is indeed unavoidable in this region.

In the solution of local system of equations, the traction boundary condition, Equation (2.5) is specifically imposed which cannot be applied to the solution of global finite element process. In the part of global mesh where no singularity is embedded, conventional recovery procedure is used prior to the above calculation.

Solution of Equation (2.27) is improved in comparison with the global mixed solution by the local information contained in the righthand side. The use of additional terms characterizing the deformation near the singularity needs to be considered. The simplest approach is to take the displacement as a dummy variable at stress-strain nodal points interpolated by conventional polynomial basis functions in a similar manner as the substructuring technique.

When such variables are introduced the solution procedure becomes very close to what is called the multi-grid method in the finite difference context. The overall solution flow is:

- (i) Solve the global stiffness equations for the global displacement, i.e.,

$$U := U + K^G{}^{-1}(\hat{F} - R)$$

- (ii) Recover the strain at nodes in the global finite element mesh.
- (iii) Evaluate the stress.
- (iv) Enter the inner loop and calculate the displacement quantity (used only as dummy variable) in the subelement mesh.

$$U^{(n+1)S} = U^{(n)S} + (K^S)^{-1} \{ F^S - B^S S^{(n)S} \}$$

- (v) Evaluate the subelement stress and strain.
- (vi) Check the convergence in terms of residual in the subelement mesh. If not converged, repeat from step (iv).
- (vii) Evaluate the global residual including the stresses in the subelement. If convergent, start a new increment, or otherwise repeat from step (i).

$$R := \hat{F} - B S^S$$

Through the inner loop, the global finite element mesh interact with the subelement and an accurate, high-resolution stress field is obtainable without increasing the size of global stiffness equations.

The additional coding is required to incorporate steps (iv) to (vi), which is performed by adding a element routine to handle the embedded singularities, and to allocate the core storage associated with the arrays used for the inner iteration. The size of algebraic equations used for representing the embedded singularity is limited by restrictiong the mesh pattern and the level of mesh refinement introduced through the subelement technique.

Incremental Iterative Solution Algorithms

The inelastic problem is solved through the deformation history in an incremental manner which is for a given state of displacement, strain and stress which satisfies the nonlinear algebraic equation (2.13) for a given load and displacement boundary conditions by U, E, S and F respectively.

Adaptive Load Incrementation Procedure:

For a given load increment ΔF , the increments of displacement, strain and stress denoted by ΔU , ΔE , and ΔS are determined in an iterative fashion as described in the previous section. Note in the preconditioning process the tangent stiffness K is used instead of the total stiffness equation. To follow a complicated equilibrium an automatic adjustment procedure procedure to control the size of load increment in the iterative process is introduced. The algorithm is schematically given as:

- (i) Set the residual vector $R := 0$;
Initialize the incremental displacement vector $\Delta U := 0$;
Set the iteration counter $i := 0$.
Apply the proportional load $\Delta F := \lambda F$ with r being the current load factor.

- (ii) Update the displacement

$$\Delta U := \Delta U + dU \quad (2.28)$$

with the update

$$dU := K^{-1}(F_0 + \Delta F - R) \quad (2.29)$$

being stored in the memory, where F_0 is the load vector at the beginning of the current increment.

- (iii) For a given arc-length, find the total load factor update

$$\lambda := \lambda + d\lambda \quad (2.30)$$

and the incremental load factor

$$\Delta \lambda := \Delta \lambda + d\lambda \quad (2.31)$$

based on the spherical path formulation [Crisfield (1980)].

- (iv) Modify the load

$$\Delta F := \Delta \lambda F \quad (2.32)$$

- (v) Form the residual in the mixed manner as indicated in steps (iii) to (v) in the previous flow chart. If convergent, then exit; otherwise repeat from step (ii).

BFGS Update Procedure

For the iterative process using the mixed residual vector, any iterative method to improve the convergence characteristics applicable to nonlinear finite element calculations can be used for the present approximation method. For instance, the BFGS update procedure [Matthies, Strang (1979)] is utilized in the following fashion:

- (i) Initialize the residual vector R and the incremental displacement ΔU such that

$$R := 0 ; \Delta U := 0 \quad (2.33)$$

- (ii) Modify the residual with i being the iteration counter

$$F = \prod_{k=1}^n (1 + v_k w_k^T) R \quad (2.34)$$

- (iii) Intermediate displacement update

$$dU = K^{-1} F \quad (2.35)$$

- (iv) Complete the displacement update

$$dU := \prod_{k=1}^n (1 + w_k v_k^T) dU \quad (2.36)$$

- (v) Form the new incremental displacement

$$\Delta U := \Delta U + dU \quad (2.37)$$

- (vi) Form the new residual with respect to the updated incremental displacement using steps (iii) to (v) in the first flow chart.

- (vi) Check the convergence and if necessary repeat from the step (ii) or else, exit.

Note in the above algorithm, vectors v and w represents the iterative change in the residual and the displacement vector respectively so as to form the inverse BFGS update

$$K_n^{-1} = (1 + w_n v_n^T) K_{n-1}^{-1} (1 + v_n w_n^T) \quad (2.38)$$

It is possible to introduce the combined BFGS - arc length algorithms in the mixed iterative solution algorithms incorporating the line search technique.

The Line Search Algorithm

The line search algorithm is used for the acceleration of niterative solution processes. After an update vector du for the velocity is obtained for a current displacement increment, we seek for a search distance s which approximately satisfies the orthogonality condition

$$g = \delta u^T R(u - s \delta u) = 0 \quad (2.39)$$

An iterative algorithm [Abdel Rahman (1982)] is implemented to find zero for the above defined function g of which the extrapolation procedure performed at each iteration is illustrated in Fig.2.2.

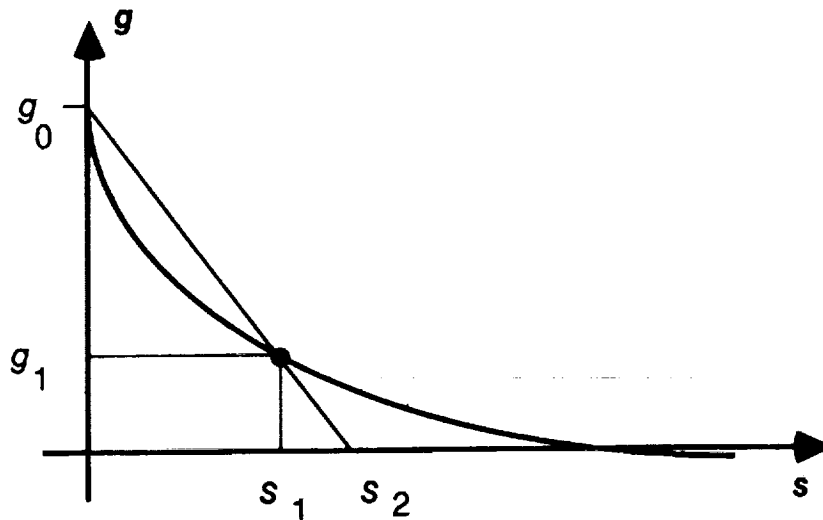


Figure 2.2 Linear Extrapolation in Nonlinear Line search

The computational procedure is schematically written as:

(i) Set $s = 1$

(ii) Recover the residual vector

$$R := R(u - s\delta u) \quad (2.40)$$

(iii) Inner product to evaluate the function

$$g = \delta u^T R \quad (2.41)$$

(iv) If $g \leq \epsilon$ a predefined tolerance then exit; else:

(v) Extrapolate linearly the search distance such that

$$s := s - \frac{g}{g - g_0} s \quad (2.42)$$

(vi) If $s \geq s_0$, with s_0 being the prescribed upper bound, set $s = s_0$.

Formulation of Finite Deformation Analysis Procedure with Particular Emphasis on Plasticity

The formulation and algorithm for the analysis of finite deformation problem implemented in the MHOST mixed iterative method is described in this subsection. The formulation utilizes the kinematics of updated Lagrangian concept. The choice of deformation and stress measures in the finite deformation analysis depends primarily on the form of the constitutive description involved, along with the necessity that the measures are objective for rigid body motions. For elastic-plastic behavior where the response depends primarily on the current state of stress, a Cauchy stress and rate-of-deformation constitutive formulation is frequently the most convenient choice.

The constitutive integration algorithms in the updated Lagrangian formulation is essentially the same as those used for infinitesimal deformation calculations, with the exception that all tensors and integrals are evaluated with respect to the current configuration. The present version of this update strategy utilizes the nodal coordinates updated continuously during the iterations in conjunction with the deformation gradient evaluated simultaneously at nodes.

We shall now summarize the iterative solution algorithm for an increment. Following initialization, the process is repeated iteratively until the equilibrium has been satisfied.

(i) Initialization:

$$U^i = U^{i-1} \quad S^i = S^{i-1} \quad R := F \quad (2.43)$$

(ii) Equation Formulation and Displacement Solution:

$$\Delta U^i = K^{-1} R^i \quad (2.44)$$

(iii) Update Geometry:

$$x^{i+1} = x^i + \Delta U^i \quad (2.45a)$$

$$U^{i+1} = U^i + \Delta U^i \quad (2.45b)$$

$$\mathcal{F}_{rel}^{i+\frac{1}{2}} = I + \nabla \left(\frac{1}{2} \Delta U^i \right) \quad (2.45c)$$

$$\mathcal{F}_{rel}^{i+1} = I + \nabla(\Delta \mathbf{U}^i) \mathcal{F}^{1+\frac{1}{2}} = \mathcal{F}_{rel}^{i+\frac{1}{2}} \mathcal{F}^i \quad (2.45d)$$

$$\mathcal{F}^{1+1} = \mathcal{F}_{rel}^{i+\frac{1}{2}} \mathcal{F}^i \quad (2.45e)$$

$$\mathcal{R}^{i+\frac{1}{2}} = \mathcal{F}^{i+\frac{1}{2}} \left(\mathcal{U}^{i+\frac{1}{2}} \right)^{-1} \quad (2.45f)$$

$$\mathcal{F}^{1+1} = \mathcal{F}_{rel}^{i+\frac{1}{2}} \mathcal{F}^i \quad (2.45g)$$

$$\mathcal{R}^{i+1} = \mathcal{F}^{i+1} \left(\mathcal{U}^{i+1} \right)^{-1} \quad (2.45h)$$

(iv) Strain Projection:

$$\Delta \mathbf{E}^{i+1} = \left(\mathbf{C}^{i+1} \right)^{-T} \mathbf{B}^{i+1} \Delta \mathbf{U}^i \quad (2.46)$$

(v) Stress Recovery:

$$\mathbf{S}_R^{i+1} = \mathbf{D}_R^{i+1} \left(\mathcal{R}^{i+\frac{1}{2}} \right)^T \Delta \mathbf{E}^{i+1} \mathcal{R}^{i+\frac{1}{2}} + \mathbf{S}^i \quad (2.47)$$

(vi) Rotate Back to Global System: For stress components

$$\mathbf{S}^{i+1} = \mathcal{R}^{i+\frac{1}{2}} \mathbf{S}_R^{i+1} \left(\mathcal{R}^{i+\frac{1}{2}} \right)^T \quad (2.48a)$$

and for plastic strain components, we have

$$\left(\mathbf{E}_{PL} \right)^{i+1} = \mathcal{R}^{i+1} \left(\mathbf{E}_{PL} \right)_R^{i+1} \left(\mathcal{R}^{i+1} \right)^T \quad (2.48b)$$

Material tangent is updated as

$$\left(\mathbf{D} \right)^{i+1} = \mathcal{R}^{i+1} \left(\mathbf{D} \right)_R^{i+1} \left(\mathcal{R}^{i+1} \right)^T \quad (2.48c)$$

Internal variables such as the back stress is also updated by

$$\left(\mathbf{a} \right)^{i+1} = \mathcal{R}^{i+1} \left(\mathbf{a} \right)_R^{i+1} \left(\mathcal{R}^{i+1} \right)^T \quad (2.48d)$$

(vii) Form Residual:

$$R^{i+1} = \int_{\Omega^{i+1}} (N^{i+1})^T f^{i+1} N^{i+1} dx^{i+1} - B^{i+1} S^{i+1} \quad (2.49)$$

If converged exit, else update displacement via line search or displacement solution and repeat. In the finite displacement calculations, the stiffness array is assembled in the following manner and repeatedly updated in the iteration loop unless other iteration process (modified-, quasi-, or secant-Newton option) is specified. Note that this stiffness matrix update does not correspond to the classical Newton method in the mixed iterative solution framework because of the independent C^0 -continuous stress interpolation functions with K being the index for nodes,

$$\sigma^h = N_K S_K \quad (2.50)$$

Whenever the stiffness matrix is reformulated in an updated Lagrangian algorithm, the shape functions, derivatives of the shape functions and determinants of Jacobians are evaluated with the nodal coordinates of the current configuration. In addition, the material and stress matrices are also the values computed in the immediately preceding iteration.

Semidiscrete Finite Element Equations and Temporal Discretization

The finite element equations of dynamic equilibrium for a deformable body is written in terms of nodal acceleration vector a , nodal velocity vector V and nodal stress vector S as

$$Ma + CV + BS = F \quad (2.51)$$

where M is the mass matrix defined by

$$M = \rho \int_{\Omega} N^T N dx \quad (2.52)$$

with ρ and N being the material density and the vector of interpolation functions, respectively. The damping matrix C may be defined as a linear combination of mass and stiffness matrices, M and K , such that

$$C = p_1 M + p_2 K \quad (2.53)$$

with p_1 and p_2 being preassigned constants representing the effects of viscous and structural damping, respectively. Symbolically, the stiffness matrix can be written by

$$K = \int_{\Omega} (\nabla N)^T D \nabla N dx \quad (2.54)$$

with E being the gradient operator and D the material modulus. The third term in Equation (2.47) represents the internal energy with B matrix being the discrete gradient operator defined in the finite element approximation subspace such that

$$B = \int_{\Omega} (\nabla N)^T N dx \quad (2.55)$$

Note that this array differs from usual displacement-strain matrix in conventional finite element computations.

Here the equal order interpolation using the same basis function is assumed for the acceleration, velocity, displacement, and stress. Introducing the process to recover the nodally interpolated strain by

$$E = GBU \quad (2.56)$$

where G is the diagonalized gramm matrix of which l th diagonal entry is calculated by

$$G = \sum_{K=1}^{N_{node}} \int_{\Omega} (N_K)^T N dx \quad (2.57)$$

with N_{node} being the total number of nodes in a mesh. Then the stress is recovered at nodes.

Note that all the integration appeared in the above equations are evaluated approximately using the numerical quadrature. The particular choice of the numerical integration rule is discussed in the subsection of element formulation.

Now we construct an abstract iterative process for the semi-discrete Equations (2.52) using the displacement preconditioning. The approximation of internal energy by the product of stiffness matrix and total displacement vector u leads to a recursive expression

$$Md^{j+1} + CV^{i+1} + KU^{i+1} = F - (BS^i - KU^i) \quad (2.58)$$

with subscripts denoting the iteration counter. For the linear elastic problem, the displacement converges linearly for an appropriate initial condition such as $U = 0$.

Note that the strain projection procedure and stress recovery operation, Equations (2.56) and (2.58), are executed every time when the displacement vector is updated.

The fully discretized system of equations is derived for the mixed iterative solution by introducing the temporal approximation. For the sake of simplicity and clarity when it is implemented, the Newmark family of algorithms is introduced in a finite difference fashion e.g., HUGHES (1984) such that the dynamic equilibrium is satisfied at time $t + \Delta t$

$$M a_{t+\Delta t} + C V_{t+\Delta t} + B S_{t+\Delta t} = F_{t+\Delta t} \quad (2.59)$$

which leads to a time discrete displacement preconditioning

$$\begin{aligned} M a_{t+\Delta t}^{i+1} + C V_{t+\Delta t}^{i+1} + K U_{t+\Delta t}^{i+1} \\ = F - (B S_{t+\Delta t}^i - K U_{t+\Delta t}^i) \end{aligned} \quad (2.60)$$

and the updates for displacement and velocity are given by

$$U_{t+\Delta t}^i = U_t + \Delta t V_t + \frac{\Delta t^2}{2} \{ (1 - 2\beta) a_t + 2\beta a_{t+\Delta t}^i \} \quad (2.61a)$$

$$V_{t+\Delta t}^i = V_t + \Delta t \{ (1 - \gamma) a_t + \gamma a_{t+\Delta t}^i \} \quad (2.61b)$$

Introducing

$$\Delta U_t^i = U_{t+\Delta t}^i - U_t \quad (2.62a)$$

and

$$\delta U_t^i = \Delta U_t^{i+1} - \Delta U_t^i \quad (2.62b)$$

we obtain a recursive form

$$\left\{ \left(\frac{1}{\beta \Delta t^2} \right) M + \left(\frac{\gamma}{\beta \Delta t} \right) C + K \right\} \delta U_t^i$$

$$\begin{aligned}
&= F_{t+\Delta t} - \left[B S_{t+\Delta t}^i + \left\{ \left(\frac{1}{\beta \Delta t^2} \right) M + \left(\frac{\gamma}{\beta \Delta t} \right) C \right\} \Delta U_t^i \right] \\
&+ \left(\frac{\gamma}{\beta} - 1 \right) C V + \left(\frac{\gamma}{2\beta} - 1 \right) \Delta t C a_t + \left(\frac{1}{\beta \Delta t} \right) M V_t + \left(\frac{1}{2\beta} - 1 \right) M a_t \quad (2.63)
\end{aligned}$$

with the incremental displacement Δu being updated by

$$\Delta U_t^i = \Delta U_t^i + \delta U_t^i \quad (2.64)$$

and the incremental strain recovered at node by

$$\Delta E_{t+\Delta t}^i = G^{-1} B^T \Delta U_{t+\Delta t}^i \quad (2.65)$$

In a general setting of history dependent inelastic constitutive integration, the stress recovery process is written as

$$S_{t+\Delta t}^i = S + \int_0^{\Delta E_{t+\Delta t}^i} S dE \quad (2.66)$$

which is fed into the equilibrium iteration defined by Equation (2.63).

Computational effort involved in the above iterative process for direct time integration of the discrete equation of motion is the assembly of element operator matrices appear in the left-hand side of Equation (2.63). This is exactly the same amount of effort required to solve the problem by the conventional displacement method. Additional computation required for the mixed solution is a few back substitution and strain and stress recovery at nodes which are relatively inexpensive compared with the matrix assembly and factorization. This additional computational cost would vanish when the scheme is applied to nonlinear problems. The matrix assembly and factorization or back substitution needs to be performed repeatedly no matter which finite element method is used to drive the solution. Therefore, seemingly complicated derivation of the mixed iterative solution scheme does not increase the computational effort in comparison with the displacement formulation to fully enjoy the advantages of equal order interpolation of displacement, strain and stress.

With particular application to turbo machinery blades and other rotating structures, the stiffness matrix is modified to include the effects of stress stiffening and centrifugal mass terms. These are linearized models of large displacement and follower force around a given state of stress due to the linear elastic response of

structures under a given angular velocity.

The centrifugal load vector is generated by integrating the body force

$$F_0 = \int_{\Omega} N \rho \omega^2 r(x) dx \quad (2.67)$$

with ω being the angular velocity and r the distance between the point and the axis of rotation. Under the centrifugal loading given above, the mixed iterative algorithm results in a certain stress field represented by the nodal stress vector s such that the discrete equilibrium equation is satisfied. Our interest is to calculate the linearized response of structure under the state of stress given by S^0 . Taking the initial stress terms into account, the equilibrium equation is modified (excluding the damping term) to

$$Ma + K_G^0 U + B^T S = F \quad (2.68)$$

where K is the geometric stiffness term associated with the initial stress field s given by

$$K_G^0 = \int_{\Omega} \nabla N^T S \nabla N dx \quad (2.69)$$

Note that Equation (2.64) is a general expression for the linearized response of structural systems under a prescribed initial stress field.

When this term is included in the mixed iterative computations, the abstract recursive form, Equation (2.55) is modified to

$$Ma + (K_G^0 + K)U_{i+1} = F - (B^T S_i - (K_G^0 + K)U_i) \quad (2.70)$$

or in terms of displacement update

$$(K_G^0 + K)U_{i+1} = F - (B^T S_i - K_G^0 U_i) \quad (2.71)$$

with

$$U_{i+1} = U_i + \Delta U_i$$

In the residual force calculations, the initial stress matrix needs to be evaluated

repeatedly with the stress field calculated at the beginning of the increment.

The additional force due to the relative motion from the equilibrium position referred to as the centrifugal mass term is also added to the equilibrium equation resulting in

$$M a + (K_G^0 - M_C) U_{i+1} + B^T S = F \quad (2.72)$$

where M is the centrifugal mass matrix defined by

$$M_C = \int_{\Omega} \rho \omega^2 N^T L N dx \quad (2.73)$$

with L being the matrix of unit vector m parallel to the axis of rotation given by

$$L = \begin{bmatrix} m_2^2 + m_3^2 & -m_1 m_2 & -m_3 m_1 \\ -m_1 m_2 & m_3^2 + m_1^2 & -m_2 m_3 \\ -m_3 m_1 & -m_2 m_3 & m_1^2 + m_2^2 \end{bmatrix} \quad (2.74)$$

Note that when this term is activated in the quasi-static and transient dynamic computations, the same correction of the residual vector calculation as for the stress stiffening terms as indicated in the right-hand side of Equation (2.71).

Typically, these optional terms are activated for the vibration analysis of rotating structures by extracting the modes from an eigenvalue problem

$$\{M - \lambda(K_G^0 - M_C + K)\} X = 0 \quad (2.75)$$

In the modal analysis, the displacement preconditioner is assumed to represent the stiffness of structures. However, the stress data used in the evaluation of initial stress terms are calculated by the mixed iterative method which generates more accurate stress field than the conventional displacement method. Hence, the solution of Equation (2.75) is expected to be somewhat more accurate than the displacement method solution.

For the detail of the derivation of initial stress and centrifugal mass matrices and fully worked out examples, see THOMAS, MOTA, SOARES (1973), RAWTANI, DOKANISHI (1974).

Additional Remarks

In the present implementation of mixed iterative solution, the displacement stiffness equations need to be assembled and factorized. To enhance the efficiency of MHOST code, the profile solver replaces the constant bandwidth Crout decomposite algorithm. The implementation of solver is based on the code published by TAYLOR (1985). The code presented in the paper include both symmetric and non-symmetric cases using the Crout decomposition. The implementation of MHOST code excludes the nonsymmetric part of code to gain the maximum efficiency. The profile storage of the global stiffness equations reduces the memory requirement and time required for factorization. Computational overhead is added to prepair the elimination table for a stiffness matrix stored in profile form.

In the quasi-static computations, option added to accelerate the rate of convergence for nonlinear iterations are made functional incorporating with the profile solver. These options are the modified Newton, quasi-Newton method of inverse BFGS update, secant Newton implementation of Davidon rank-one quasi-Newton update, conjugate gradient and line search. The spherical path version of arc length method incorporating with the modified Newton iteration is also made available for the profile solver.

The eigenvalue extraction procedure implemented in the MHOST code is based on the subspace iteration documented by BATHE, WILSON (1976). In this process, a large eigenproblem of structural systems is mapped into a subspace of finite dimensions and the Jacobi iteration is performed to solve the small eigenproblem set in the subspaces. This eigenvalue extraction procedure is used to compute the natural frequency and vibration mode of unstressed and prestressed structures and the buckling analysis of prestressed structures undergoing elastic or inelastic deformation of infinitesimal or finite amplitude.

Note here that in the eigenvalue extraction, the displacement stiffness matrix is used to represent the response of structural systems. However, in the buckling and model analyses with prestress, the improvement of stress field generally improves the quality of solution considerably. The utilization of mixed stress interpolation in the eigenvalue analysis can be viewed as a perturbed eigenvalue problem in which the effect of independent stress approximation is regarded as the perturbation to the displacement finite element system. It is anticipated that an algorithm proposed by SIMO (1985) and implemented for the NESSUS probabilistic finite element code may be usable for eigenvalue extraction of mixed system of finite element equations.

3. ELEMENT TECHNOLOGY

Introductory Remarks

The MHOST program consists of a library of highly accurate linear quadrilateral and hexahedral elements. The selective reduced integration and assumed stress interpolation are used to improve the element responses under bending load. To take the full advantage of these formulations, a rational local coordinate transformation derived from the polar decomposition of the Jacobian matrix is developed and implemented in the code. This highly sophisticated algorithm makes the response of element insensitive to the isoparametric distortion.

For the sampling and nodal projection of element strain components, the trapezoidal integration rule is utilized for the maximum accuracy and stability. The oscillation of strain/stress fields often observed at the element integration points are filtered out by this procedure. The resulting mixed iterative finite element method is capable of producing very accurate displacement, strain and stress simultaneously.

The nodally continuous stress assumption used in the beams and shells improves the accuracy of MHOST solution considerably in comparison with the conventional displacement strategies. For example, the nodally exact displacement and moment solution is obtained for a cantilever beam problem modelled by the MHOST shell element subjected to a point load in the transverse direction at the tip. This shows the capability of the mixed iterative shell formulation to capture the linear moment field exactly by using only the linear finite element basis functions.

To avoid numerical instabilities commonly observed for the four node shell elements such as the *numerical locking* and *hourglass* displacement modes, the stiffness matrix for the shell element uses the selective integration for the transverse shear terms and a simple and efficient hourglass control scheme proposed by BELYTSCHKO, TSAY & LIU (1981).

The sophisticated three dimensional element implemented in the MHOST program exhibits superior accuracy in comparison with the conventional isoparametric 8 node brick element derived directly from the displacement method formulation. The selective shear integration/assumed stress formulation in conjunction with the local coordinate transformation based on the isoparametric

mapping results in a highly accurate displacement field even at the initial displacement preconditioning phase without iterative improvement. The iterative process drives the solution further toward the direction of high accuracy for the given mesh.

To generate a good displacement update for preconditioning purposes, two major refinements are incorporated in the present computational procedure. These are the improved version of filtering scheme for the selectively reduced integration and the modified numerical quadrature for plates and shells to avoid possible kinematic mode excitation.

Coordinate Transformation and Filtering Algorithms

An element coordinate system is developed in this section which neutralize the rotation associated with the isoparametric representation of the element. The procedure is similar to the kinematics of finite deformation processes. It is developed to handle two- and three-dimensional elements in a unified manner.

The isoparametric transformation is defined by the Jacobian

$$J = \left[\frac{\partial x_i}{\partial \Xi_j} \right]$$

where x denotes the *physical* coordinate vector with X being the reference (isoparametric) coordinate system. The isoparametric transformation is decomposed to the rotation and stretch by virtue of the polar decomposition

$$J = RU$$

where R denotes the rotation tensor with U being the right stretch tensor with respect to the isoparametric mapping. The rotation tensor is calculated by

$$R = JU^{-1}$$

Using this orthogonal tensor, the rotation neutralized coordinate system X is defined by

$$X = g x$$

or, by using the indicial notation,

$$X^m = g_k^m x_k$$

where

$$g = R^{-1}$$

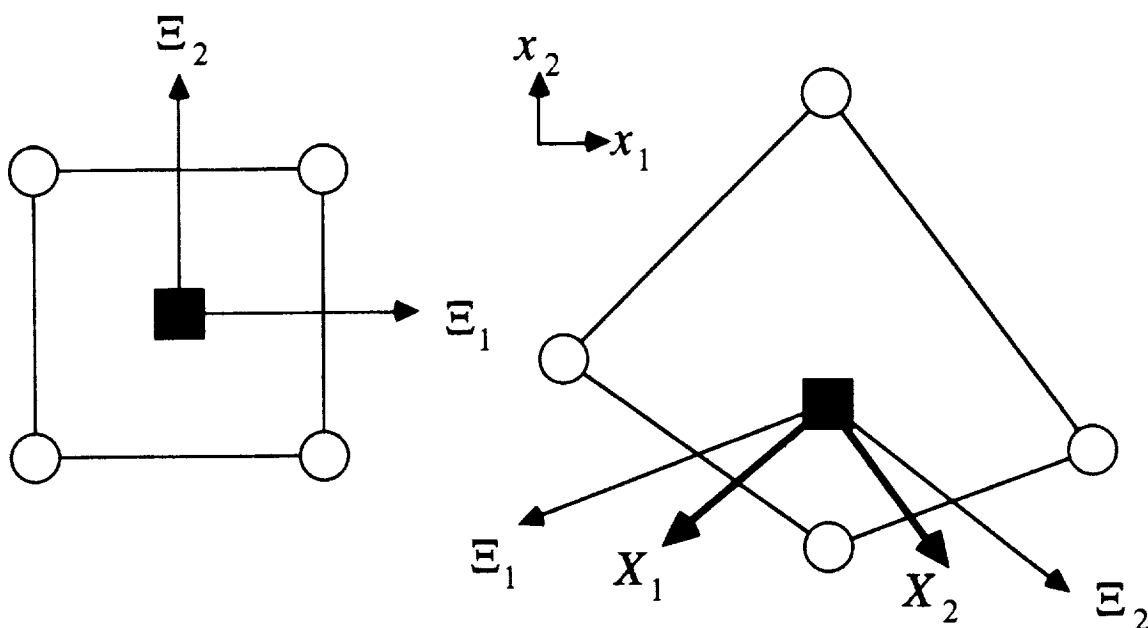
The figure depicts the definition of coordinate systems used in this development. In order to maintain the flexibility in the development of numerical integration procedures for element arrays, the operation is carried out only at the element centroid. The coordinate system defined at the element centroid is used for the definition of vector and tensor components in the element.

The right Cauchy deformation tensor is defined by a product of Jacobian as

$$C = J^T J$$

or alternatively, in terms of the right stretch tensor

$$C = U^T U$$



a) The Parent Element in the Isoparametric Space

b) A Typical Element in the Physical Plane

Figure 3.1 Definition of Coordinate Systems for a Linear Isoparametric Element in Two Dimensions

In terms of the right Cauchy deformation tensor, the right stretch tensor is expressed

as

$$U^{-1} = C^{-\frac{1}{2}} = N_C^T \lambda_C^{-\frac{1}{2}} N_C$$

Hence, the rotation tensor is calculated from the expression

$$R = J \left(N_C^T \lambda_C^{-\frac{1}{2}} N_C \right)$$

Eigenvalues and eigenvectors of the right Cauchy-Green tensor are calculated by using the Cayley-Hamilton formula in two dimensions whereas an iterative process is used for the three dimensional application of this coordinate transformation. The Cayley-Hamilton formula used in the polar decomposition. is given as

$$U = \frac{1}{\sqrt{I_C + 2\sqrt{II_C}}} (C + \sqrt{II_C} I)$$

where

$$I_C = \text{trac} C, II_C = \det C,$$

and

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The kl -th component of the linear infinitesimal strain tensor in the local coordinate system $\epsilon^{(kl)}$ is written in terms of components in the global coordinate system such that

$$\epsilon_{ij}^{(kl)} = g_i^{(k)} g_j^{(l)} \epsilon^{(kl)}$$

Summation is not implied the superscripts in the parentheses. Using the strain components in the global coordinate system, we have the strain component defined in the local coordinate system by

$$\epsilon^{(kl)} = g_m^{(k)} g_n^{(l)} \epsilon_{mn}$$

Hence the ij -th strain component can be represented by the product of coordinate transformation and the original global strain components by

$$\epsilon_{ij}^{(kl)} = g_i^{(k)} g_j^{(l)} g_m^{(k)} g_n^{(l)} \epsilon_{mn}$$

It is interesting to note that, the full coordinate transformation system is an identity tensor

$$g_i^{(k)} g_j^{(l)} g_m^{(k)} g_n^{(l)} = I$$

Introducing the *filtering matrix* for the selective integration defined by

$$G_{ij}^{(k)} = g_i^{(k)} g_j^{(k)}$$

The strain component in the local coordinate system can be written in a simpler manner

$$\epsilon_{ij}^{(kl)} = G_{im}^k G_{jn}^l \epsilon_{mn}$$

The volumetric strain in the element coordinate system is defined as

$$\begin{aligned} \epsilon^{(v)} &= \epsilon^{kk} \\ &= G_{im}^k G_{jn}^l \delta^{kl} \epsilon_{mn} \end{aligned}$$

Similarly the deviatoric strain components in the element coordinate system is written as

$$\begin{aligned} \epsilon^{(d)} &= \epsilon^{kk} \\ &= G_{im}^k G_{jn}^l (1 - \delta^{kl}) \epsilon_{mn} \end{aligned}$$

In the numerical integration process, at the full integration points we evaluate

$$\epsilon = \alpha \epsilon^{(v)} + \beta \epsilon^{(d)}$$

whereas at the reduced integration point,

$$\epsilon = (1 - \alpha) \epsilon^{(v)} + (1 - \beta) \epsilon^{(d)}$$

typically with

$$\alpha \approx 1 ; \beta \approx 0$$

This effectively filters the spurious bending stiffness associated with the linear isoparametric element formulation based on the conventional displacement formulation.

Defining the original strain component E by

$$E = BU \quad (3.15)$$

with B being the usual strain-displacement matrix calculated at the quadrature points and U the nodal displacement vectors, the energy functional $I(U)$ is obtained in terms of nodal displacement for linear elasticity as an example by,

$$I(U) = \frac{1}{2} \left\{ \int_{\Omega} \lambda E^{(v)} \otimes E^{(v)} dx + \int_{\Omega} \mu E^{(d)} \otimes E^{(d)} dx \right\} - \int_{\Omega} F \cdot U dx - \int_{\partial\Omega} T \cdot U ds \quad (3.16)$$

where \otimes denotes tensor inner products, λ and μ are the Lamme-Navier coefficients and F and T are the prescribed body force and surface traction respectively.

In the above energy functional, either the first term or the second term is under-integrated to realize the necessary effects of the selectively reduced integration.

In computations, it is often more convenient to construct the strain-displacement matrix selectively, so that the above energy functional can be written as

$$I(U) = \frac{1}{2} U^T \int_{\Omega} B_S^T D B_S dx U - F^T U \quad (3.17)$$

where F is the collection of prescribed load terms which appeared in equation (2.48). The new strain-displacement matrix B is the selectively sampled matrix equivalent to a certain mixed method under the isoparametric distortion. In the matrix notation, the filter for the element volumetric strain is written as

$$E^{(V)} = G^T IGBU \quad (3.18)$$

and for the element deviatoric strain

$$E^{(D)} = G^T(1 - I)GBU \quad (3.19)$$

at each integration point, with 1 and I being matrices

$$1 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} ; \quad I = \delta_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (3.20)$$

Hence, we have

$$B_S = G^T IGB + G^T(1 - I)GB \quad (3.21)$$

where either the first or the second term is sampled at the reduced integration points and substituted to the array associated with the full integration points. Such an operation is trivial only for the linear Lagrangian elements with a single reduced integration point.

Hourglass Control Algorithm for Plates and Shells

The kinematic model generated by the reduced integration of transverse shear terms in the 4 noded bilinear plates and shell elements often induce numerical noise in the displacement preconditioning operation. However, excitation of these modes often referred to as the hourglass mode does not significantly deteriorate the convergence of the mixed iterative algorithms. To eliminate these modes filtering methods have been developed either to constrain the modes by modifying the stiffness equation (a priori hourglass control) [BELYTSCHKO, FLANAGAN (1982)] or to filter out the spurious noise after the nodal displacement is obtained (a posteriori hourglass control) [ODEN (1983)].

Noting that the fully integrated stiffness matrix does not contain the kinematic modes, we utilize a simple version of a priori hourglass control algorithm originally developed by BELYTSCHKO et.al. (1982). Note also that the fully integrated equation locks the structure which produces excessive strain energy associated with the transverse shear terms for a given displacement field.

Constructing the transverse shear stiffness matrix K by adding

$$K_S = \epsilon K_S^{(2x2)} + (1 - \epsilon) K_S^{(2x2)} \quad (3.22)$$

where ϵ is the parameter associated with the aspect ratio of the element, the

kinematic mode can be eliminated without the expense of numerical locking, due to the insignificant participation of the fully integrated terms.

The formula to calculate the filtering participation of K is calculated at the centroid of the element such that

$$\varepsilon = \varepsilon_0 t_C / h \quad (3.23)$$

with t being the thickness of the element at the centroid and h is the mesh size

$$h = \frac{1}{2}(|x_1 - x_4| + |x_2 - x_3|) \quad (3.24)$$

Typically $\varepsilon_0 = 0.01$ is used for the validation and verification exercises.

No additional computational cost is involved in this hourglass control algorithm because the element stiffness equations are integrated selectively and K is readily available without adding a new integration procedure.

Assumed Stress Element Formulations

In order to boost the performance of continuum elements, a family of assumed stress element formulations is added in the mixed iterative solution procedure. Regular continuum elements often lack the appropriate deformation modes to model shell-like structures in a satisfactory way. This was observed by AHMAD, ZIENKIEWICZ (1972) in the development of the 8-node thick shell element. The problem was circumvented by a selective reduced integration formulation. There are a class of shell elements incorporating special interpolations for the transverse shear terms to retain accuracy for the bending behavior of shells, e.g., Heterosis element of HUGHES, TEZDUYAR (1978) and the 8 and 9-node thick shell elements proposed by HINTON, HUANG(1986). Four and eight node versions of such elements are proposed by NAGTEGAAL, NAKZAWA, TATEISHI (1987).

The original library of continuum elements implemented in MHOST (element types 3, 7, 10 and 11) are based on the selective reduced integration with the coordinate transformation in order to retain invariance with respect to the isoparametric transformation. In recent paper by PIAN, SUMIHARA (1986), a *hybrid stress* element which exhibits excellent bending behavior for distorted configurations. The element uses five independent stress parameters to define the element stress field.

The assumed stress element formulation developed in this program is a family of continuum-type elements with enhanced bending behavior with

reasonable accuracy even at a high aspect ratio. The elements were constructed using an assumed strain formulation. The basic strategy is: (i) the identification of a set of independent stress modes representing the desired element behavior, (ii) the construction of a corresponding set of strain modes which results in a proper set of stress modes. The formulation is the conventional strain-driven form and implemented in the existing MHOST framework for material nonlinear problems. The strain modes are used to interpolate the element strain field and are projected to the displacement gradients by a mean square manner. All assumed strain modes are expressed in terms of a local element cartesian coordinate system obtained by polar decomposition of the isoparametric mapping at the centroid of the element. The stretch tensor obtained in the polar decomposition is used for computing scale factors to make the element computation dimensionless.

The library of assumed strain elements implemented in MHOST includes 4-node quadrilaterals for plane strain, plane stress and axisymmetric problems, and an 8-node solid element for modeling three-dimensional continua. The current implementation can be used with either the displacement or the mixed formulation and supports different integration rules for strain projection and residual recovery.

Additional Remarks

An algorithm is adapted in MHOST to allow the nodal definition of pressure loading on 2 and 3D continuum meshes. The algorithm is based on a nodal assembly of tributary areas at each node in such a way that a unique outward boundary normal vector is defined at each surface node. These normals define the effective surface orientation and the direction of the applied pressure at the node.

For small deformation problems, this operation is carried out only once, during the first element assembly loop, and the resulting boundary normals are used to compute consistent pressure loads throughout the analysis.

4. ITERATIVE SOLUTION ALGORITHMS

Introductory Remarks

In this section, iterative solution algorithms used for the solution of mixed finite element equations are discussed in detail. The fundamental solution strategy is presented in the following flow chart. This process is similar to the modified Newton approach for the nonlinear finite element calculations. One can find similarity of the process to the Uzawa's algorithm for constrained minimization problems.

Step 1: Initialization

$$\mathbf{r}^n = \mathbf{f} \quad \text{and} \quad \mathbf{u}^n = 0$$

Step 2: Nodal displacement update

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \mathbf{K}^{-1} \mathbf{r}^n$$

Step 3: Strain projection to the nodes

$$\boldsymbol{\varepsilon}^{n+1} = \mathbf{C}^{-1} \mathbf{E} \mathbf{u}^{n+1}$$

Step 4: Stress recovery at the nodes

$$\boldsymbol{\sigma}^{n+1} = \mathbf{C}^{-T} \mathbf{G} \boldsymbol{\varepsilon}^{n+1}$$

Step 5: Form the residual

$$\mathbf{r}^{n+1} = \mathbf{f} - \mathbf{E}^T \boldsymbol{\sigma}^{n+1}$$

If $\|\mathbf{r}^{n+1}\| > \text{tolerance}$ go to Step 2.

where notation defined in the first section is used to identify vectors and matrices appeared in the mathematical expressions.

The displacement stiffness matrix \mathbf{K} is used algorithmically to (a) obtain the

initial trial solution used to start the iterative procedure for the mixed problem, and (b) help iterate the intermediate results towards the "exact" solution for the mixed system of equations.

The Davidon Rank-one Secant Newton Update Procedure

The role of the displacement stiffness K in the solution of the mixed problem is essentially algorithmic. Therefore, we can use a simple update procedure to try to *improve* our matrix between iterations. One of the simpler procedures of this type is known as the Davidon rank-one secant Newton update. This procedure is equivalent to replacing the K matrix in Step 2 of the basic algorithm by an iteratively updated matrix of the form

$$K_{n+1}^{-1} = K_n^{-1} + \frac{(\mathbf{du}^n - K_n^{-1} \gamma^n) \otimes (\mathbf{du}^n - K_n^{-1} \gamma^n)}{(\mathbf{du}^n - K_n^{-1} \gamma^n) \cdot \gamma^n}$$

where

$$\gamma^n = \mathbf{r}^n - \mathbf{r}^{n-1}$$

i.e., the difference between the residual vectors obtained for two consecutive iterations. Of course, this is *not* how we do it in the program! As we shall see, there is a far more efficient way of programming this method.

The best way of programming this algorithm will involve only a *small number* of additional *vector operations* when the displacement updates are computed. Using this approach, we will not even need to explicitly store the update vectors employed by the algorithm! An efficient implementation of the Davidon algorithm can be summarized as follows:

Step 1: Initialization

$$\mathbf{r}^n = \mathbf{f} \quad \text{and} \quad \mathbf{du}^{n-1} = \mathbf{du}^{n-1} * = 0$$

Step 2a: Solve for the trial displacement

$$\mathbf{du}^n = K^{-1} \mathbf{r}^n$$

Step 2b: Compute the following terms

$$\gamma^n = \mathbf{r}^n - \mathbf{r}^{n-1}$$

$$c = \frac{(\mathbf{du}^{n-1*} + \mathbf{du}^n - \mathbf{du}^{n-1}) \cdot \mathbf{r}^{n-1}}{(\mathbf{du}^{n-1*} + \mathbf{du}^n - \mathbf{du}^{n-1}) \cdot \boldsymbol{\gamma}^n}$$

$$b = -c$$

$$a = 1 - c$$

Step 2c: Update the nodal displacements

$$\mathbf{du}^{n*} = a \mathbf{du}^n + b \mathbf{du}^{n-1*} + c \mathbf{du}^{n-1}$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \mathbf{du}^{n*}$$

Step 3: Strain projection to the nodes

$$\boldsymbol{\varepsilon}^{n+1} = \mathbf{C}^{-1} \mathbf{E} \mathbf{u}^{n+1}$$

Step 4: Stress recovery at the nodes

$$\boldsymbol{\sigma}^{n+1} = \mathbf{C}^{-T} \mathbf{G} \boldsymbol{\varepsilon}^{n+1}$$

Step 5: Form the residual

$$\mathbf{r}^{n+1} = \mathbf{f} - \mathbf{E}^T \boldsymbol{\sigma}^{n+1}$$

If $\|\mathbf{r}^{n+1}\| > \text{tolerance}$ go to Step 2.

As we can see, the only difference from the basic algorithm is in Step 2a-c. Please notice that the first pass with the Davidon algorithm is essentially the same as in our basic algorithm. In a way, the update procedure is "turned on" by the second pass through the iteration procedure. This algorithm can also be used in conjunction with line searches. The procedure for combining the two algorithms is very straightforward, and we will not need to complicate our discussion with those details.

Solution Algorithms for Eigenvalue Problems

Eigenvalue problems arise in a number of different situations. Let's start with the very familiar *dynamic eigenvalue problem* for (small amplitude) undamped vibration of a linear elastic structure. This will give rise to a set of matrix equations

of the form

$$(\mathbf{K} - \lambda \mathbf{M}) \phi = 0$$

where \mathbf{M} and \mathbf{K} are the consistent mass and displacement stiffness matrices for the problem. When the stiffening effects due to the initial stress field and/or the centrifugal mass effects observed in rotating machinery are included, the eigenvalue problem will become

$$((\mathbf{K} + \mathbf{K}_g - \mathbf{M}_\omega) - \lambda \mathbf{M}) \phi = 0$$

where

$$\mathbf{K}_g = \int_{\Omega} \mathbf{B}^T \sigma^0 \mathbf{B} d\Omega$$

$$\mathbf{K}_\omega = \omega^2 \int_{\Omega} \rho \mathbf{N}^T \mathbf{H}^T \mathbf{H} \mathbf{N} d\Omega$$

are the geometric stiffness and the centrifugal mass matrix.

The first one of these matrices is also used to set up the *buckling eigenvalue problem* for a linear elastic structure. If the problem is linearized about the origin (the usual case), the matrix equations will be

$$(\mathbf{K} - \lambda \mathbf{K}_g) \phi = 0$$

A related eigenvalue problem comes up in nonlinear analysis when we are trying to *detect the presence* of a nearby bifurcation. This problem can be expressed by a matrix equation of the form

$$(\mathbf{K}^n - \lambda \mathbf{K}_g^n) \phi = 0$$

where

$$\mathbf{K}^n = \int_{\Omega} \mathbf{B}^T \mathbf{D}^n \mathbf{B} d\Omega + \int_{\Omega} \mathbf{B}^T \sigma^n \mathbf{B} d\Omega + \text{other possible terms}$$

$$\mathbf{K}_g^n = \int_{\Omega} \mathbf{B}^T \sigma^n \mathbf{B} d\Omega$$

are some *tangent* material and geometric stiffness matrices, both linearized *at the end* of the last load increment. The presence of a bifurcation would be indicated by the *vanishing* of one or more eigenvalues.

Finally, we must complete our list with the *deformation modes problem* which is an eigenvalue problem of the form

$$(\mathbf{K} - \lambda \mathbf{I}) \phi = 0$$

where \mathbf{I} is an identity matrix with the appropriate rank. This problem may be used to assess the quality of the finite element approximation for certain classes of problems. It hardly ever is used in actual engineering practice.

The subspace iteration procedure is employed in the MHOST finite element program to solve the generalized eigenvalue problem. We will present this algorithm in terms of the dynamic eigenvalue problem although, in reality, the subspace iteration algorithm can be used to solve any of the eigenvalue problems discussed in the preceding pages. The basic implementation of the subspace iteration procedure will involve the following steps:

Step 1: Select the initial trial vectors

$$\Phi^n = [\phi_1^n \phi_2^n \dots \phi_m^n]$$

Step 2: Solve for the subspace vectors

$$\mathbf{R}^n = \mathbf{K}^{-1} \mathbf{M} \Phi^n$$

Step 3: Construct the reduced eigenproblem

$$\bar{\mathbf{K}}^n = \mathbf{R}^{nT} \mathbf{K} \mathbf{R}^n$$

$$\bar{\mathbf{M}}^n = \mathbf{R}^{nT} \mathbf{M} \mathbf{R}^n$$

Step 4: Solve the reduced eigenproblem

$$(\bar{\mathbf{K}}^n - \lambda_i^n \bar{\mathbf{M}}^n) \psi_i^n = 0$$

for $i = 1, 2 \dots m$ using the Jacobi iteration method.

Step 5: Obtain the improved eigenvectors

$$\Phi^n = \mathbf{R}^n [\psi_1^n \psi_2^n \dots \psi_m^n]$$

If not converged go to Step 2

APPENDIX COMPUTER CODE ARCHITECTURE

Program Organization

The architecture of the MHOST code is schematically shown in Figure A.1. The execution supervisor routine (SUBROUTINE HOST) controls multiple analysis modules in a consistent manner. In Version 4 of the MHOST code, a pair of subroutines are added to check the consistency of the Parameter Data and to generate internal flags for the selection of analysis modules. The intention is to avoid possible occurrence of users to combine the features of the program package not the way the developers designed.

The analysis modules represents the control structure of incremental iterative algorithms implemented in the MHOST code without going into detail. The source program with comments is designed to serve as the schematic flow chart of the computational process.

The schematic flow of the element and nodal data manipulation is coded in the element assembly submodules which are entered from analysis modules. The element assembly submodules performs operations independent of element types and constitutive models. The assumptions introduced in the mechanics aspects of the formulations are explicitly coded at this level. These submodules call the librarian routines for elements and constitutive models.

The element librarian subprogram (SUBROUTINE DERIV) generates quantities unique to the element used in an analysis. The MHOST code uses the standard finite element matrix notation as in ZIENKIEWICZ(1977), ZIENKIEWICZ & TAYLOR (1990). The element specific information returned from the librarian subprogram is the strain-displacement array referred to as B matrix in the previous subsections.

The constitutive equation librarian subprogram (SUBROUTINE STRESS and BMSTRS) is designed to incorporate the nodal storage of stress and strain values. The STRESS subroutine sets up the loop over the points at which constitutive equations are evaluated. The current implementation is a nested double loop with outer loop being over the node and inner loop over the integration layer through the thickness. Note that the conventional displacement method can be recovered by

restructuring this loop in conjunction with a few minor modification in the core allocation for stresses and strains.

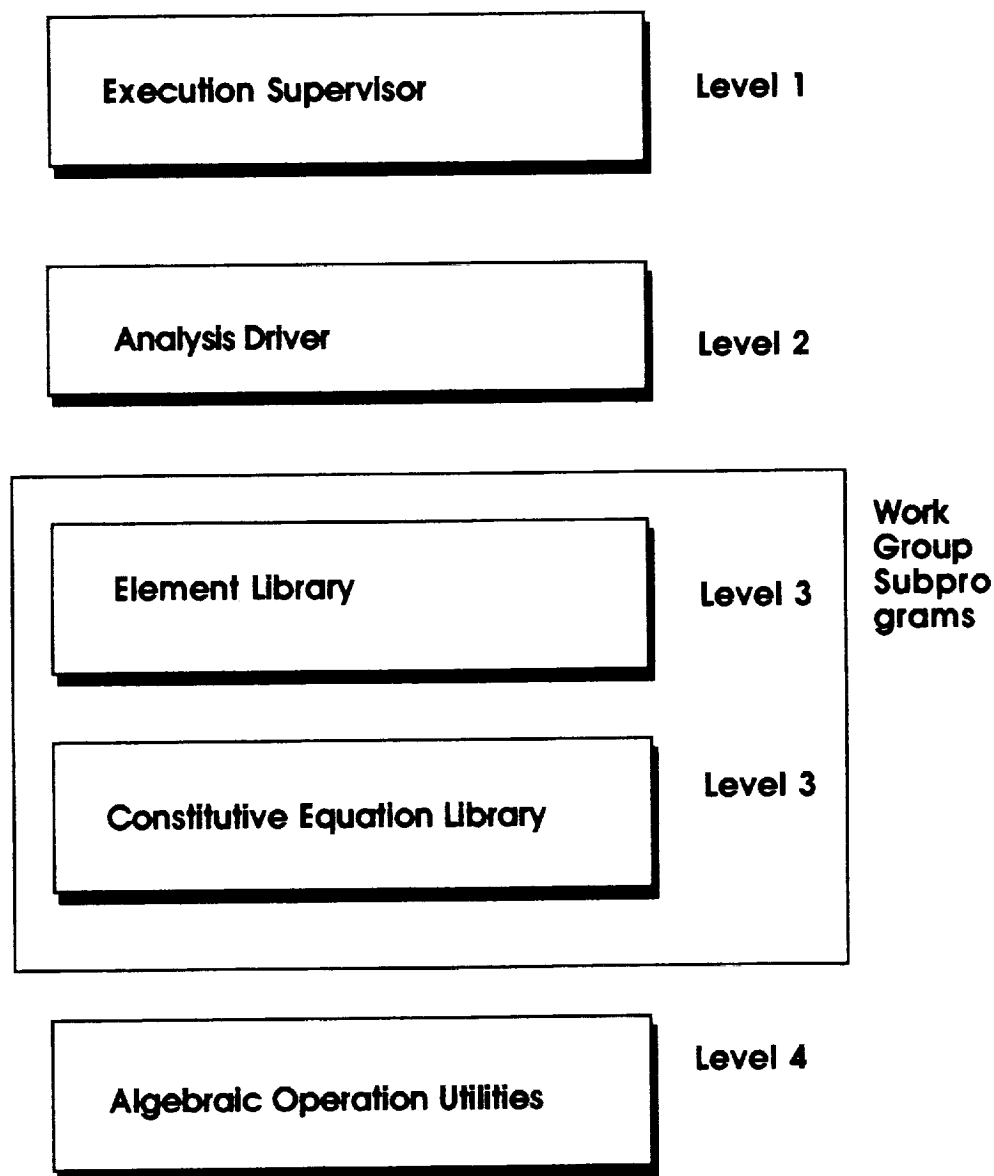


Figure 1 Organization of MHOST Program

The librarian subprogram calls the constitutive equation package (SUBROUTINE NODSTR) from which individual subprograms for initial strains, stress recovery and material tangent are called. The librarian subprograms also controls the pre-integration of stresses, strains and material tangent over thickness for the

shell element.

Note that the evaluation of the constitutive equation is one of the most costly operation in the nonlinear finite element computations. An attempt is made to minimize the execution of this process during the incremental iterative analysis, in particular the recovery of the residual vector. At the beginning of each increment, this process may be executed to evaluate the material tangent and contribution of initial strain terms which are often necessary for proper displacement pre-conditioning.

Except for a small amount of information related to the convergence of iterative solution, all the report generation is performed at the end of increment. Optionally, post-processing and restart files are written at the end of user-specified increments. Generic reporting subprograms are called from analysis modules inside of the loop over the increments.

A brief description of major subprograms are given below:

Execution Supervisor:

MAIN PROGRAM - declares the work space in blank common as an integer array. Also defines system parameters which are machine independent. Then pass the control to actual execution supervisor SUBROUTINE HOST.

SUBROUTINE HOST - controls the sequence of execution of the analysis modules. First, this routine executes the control parameter data reader SUBROUTINE DATIN1 and check the consistency by entering SUBROUTINE LETCMD and RUNCMD. The current structure of code allows certain combination of two analysis modules to be executed sequentially. Analysis modules called from the execution supervisor are:

SUBROUTINE STATIC for quasi-static incremental iterative solution.

SUBROUTINE DYNAMT for the transient time integration of dynamic equilibrium equation in an incremental-iterative manner.

SUBROUTINE MODAL for the eigenvalue extraction for vibration mode analysis. This subsystem may be executed after the quasi-static analysis for the modal analysis of prestressed structures.

SUBROUTINE BUCKLE for the eigenvalue extraction for buckling load calculation. This subsystem is executable only after the quasi-static analysis.

SUBROUTINE FRONTS for the quasi-static incremental iterative solution by

the out-of-core frontal solution. Note that certain options are not available in this subsystem.

SUBROUTINE SUPER for the linear dynamic response calculation by the method of mode superposition.

Input Data Reader :

There are three major subprograms:

SUBROUTINE DATIN1 - Reads and interprets the parameter data input called by the execution supervisor. All the default values for control variables are set in this routine.

SUBROUTINE BULKIN - Reads and interprets the finite element model definition data and prints the mesh and loading data for the initial increment (number 0). The bulk data reader is entered before the execution of analysis modules. This subroutine enters following lower level routines:

SUBROUTINE INITI1 for the memory allocation of integer workspace in the blank common to store nodal and element data.

SUBROUTINE DATIN2 for the model data input.

SUBROUTINE DATOU1 for reporting the model definition data.

SUBROUTINE CHKELM for the detection of clockwise element connectivity definition which results in the negative Jacobian matrix. This routine automatically corrects the connectivity table to counterclockwise direction.

SUBROUTINE SUBDIV for the memory allocation for the subelement mesh data and automatic mesh generation for the subelements.

SUBROUTINE INCRIN - Reads and interprets the loading and constraint data for each increment. This routine is invoked by individual analysis modules from the inside of loop over the increments.

SUBROUTINE DATIN3, a small subset of the bulk data reader SUBROUTINE DATIN1 is used for actual operations including the initialization of arrays at the beginning of increment.

Algebraic Operation Subsystem :

There are three groups of four routines for the profile solver, frontal solver and eigenvalue extraction. The profile solution package consists of:

SUBROUTINE COMPRO - Sets up the integer array for the profile of global stiffness equations to be stored in a profile form.

SUBROUTINE ASSEM5 - Assembles the element stiffness equations into the global equation system stored in a profile form.

SUBROUTINE SOLUT1 - Controls the iterative solution processes including the vector update required for the quasi- and secant-Newton iterations.

SUBROUTINE DECOMP - Factorizes the global stiffness equations stored in a profile form.

SUBROUTINE SOLVER - Performs the back substitution and generates the update vector for the incremental displacement.

The frontal solution package consists of:

SUBROUTINE FRONTW - Estimates the front matrix size to be accommodated in the core memory.

SUBROUTINE INTER - Allocates memory for the work space required for the frontal solution.

SUBROUTINE PRFRNT - Sets up the elimination table for the frontal solution.

SUBROUTINE FRONTF - Assembles and factorizes the global stiffness equation simultaneously.

SUBROUTINE FRONTB - Performs the back substitution and generates the updates for displacement vector.

SUBROUTINE FRONTR - Controls the iterative solution processes including the vector update required for the quasi- and secant-Newton iterations. Calls SUBROUTINE FRONTB for the incremental displacement update vector.

SUBROUTINE VDSKIO - Controls the data stream stored in-core buffer area and the actual out-of-core storage devices.

The eigenvalue analysis package consists of:

SUBROUTINE EIGENV - Controls the execution of eigenvalue extraction

subsystem.

SUBROUTINE INIMOP - Initializes the array for eigenvectors.

SUBROUTINE SUBSPC - Performs the subspace iteration and generates a specified number of eigenvalues and eigenvectors.

SUBROUTINE JACOBI - Solves the eigenvalue problem in the subspace by the Jacobi iteration.

There are a number of subprograms used commonly by *Algebraic Operation Subsystem*:

SUBROUTINE STRUCT - Controls the memory allocation for the global algebraic manipulations at the beginning of every analysis.

SUBROUTINE INITI2 - Allocates memory required for the storage of global stiffness matrix and other vectors required in the linear algebraic manipulation of finite element equations.

SUBROUTINE LINESR - Calculates the search distance when the line search option is turned on.

Element Assembly Submodules :

These are subprograms constructing vectors and matrices appearing in the algorithmic description of mixed iterative process discussed in the previous subsections.

SUBROUTINE ASSEM1 - Assembles the displacement stiffness matrix for the preconditioning purposes. All the options for kinematic and constitutive assumptions are treated on this module.

SUBROUTINE ASSEM2 - Assembles the coefficient matrix for the transient time integration by the Newmark family of algorithm. This routine is evolved from SUBROUTINE ASSEM1 and handles all the kinematic and constitutive options.

SUBROUTINE ASSEM3 - Assembles the coefficient matrix for the quasi-static analysis using the frontal solution subsystem. Large displacement, stress stiffening and centrifugal terms are not available in this package.

SUBROUTINE ASSEM4 - Calculates the nodal strain and recovers the residual vector in a mixed form. The subelement solution module is entered from this subprogram.

Element Loop Structure and Library Routines :

In the element assembly submodules, element arrays are generated in the loops over elements. The protocol to access to the element library is designed and implemented which involves a sequence of subroutine calls:

SUBROUTINE ELVULV - Sets up the current element parameters from the element library table.(See Table A1 for variable definition and its values)

SUBROUTINE CNODEL - Pulls out quantities for the current element from the global nodal array and restores them in the element workspace. Coordinate transformations necessary for beam and shell elements are performed in this subprogram.

SUBROUTINE DERIV - Sets up the displacement-strain matrix for the current element by calling the element library subroutines. Those are:

SUBROUTINE BPSTRS for plane stress elements, types 3 and 101.

SUBROUTINE BPSTRN for plane strain elements, types 11 and 102.

SUBROUTINE BSOLID for three-dimensional solid element, type 7.

SUBROUTINE BSHELL for three-dimensional shell element, type 75.

SUBROUTINE BAXSYM for axisymmetric solid-of-revolution elements, types 10 and 103.

SUBROUTINE BTBEAM for linear Timoshenko beam element, type 98.

SUBROUTINE BASPST for the assumed stress plane stress element, type 151.

SUBROUTINE BASPSN for the assumed stress plane strain element, type 152.

SUBROUTINE BASSOL for the assumed stress three-dimensional solid element, type 154.

SUBROUTINE UDERIV - A slot for user coded element B matrix routine.

The following subprograms are used to calculate terms appearing in the finite element equations:

SUBROUTINE LMPMAS - Calculates nodals weight factor for the strain projection.

SUBROUTINE STIFF - Performs matrix triple products to assemble the element stiffness matrix and the element load vector associated with the initial strain terms.

SUBROUTINE STRAIN - Calculates element strain at specified sampling points and projects to nodes.

SUBROUTINE CNSMAS - Assembles the consistent mass matrix for the modal and transient analysis.

SUBROUTINE INITST - Generates initial stress terms for the quasi-static, buckling and modal analysis of prestressed structures.

SUBROUTINE CENMAS - Evaluates the centrifugal mass terms for rotating structures at speed.

SUBROUTINE RESID - Calculates the element residual vector for the global element.

SUBROUTINE SUBFEM - Performs the subelement solution and calculates the element residual vector for the subelement mesh.

SUBROUTINE RELDFG - Calculates relative deformation gradient at the element sampling point and projects to node.

SUBROUTINE RESDYN - Calculates the contribution of mass and damping terms in the element residual vector when the transient dynamics option is used.

Material Library :

A system of subroutines is included in the MHOST code which covers a wide range of material models and initial strain assumptions:

SUBROUTINE SIMPLE - Integrates the stress over the increment assuming the elastic-plastic response of the material is represented by total secant modulus of elasticity. Also generates the material modulus matrix.

SUBROUTINE PLASTS - Integrates the stress over the increment and calculates the plastic strain by using the radial return algorithm.

SUBROUTINE PLASTD - Calculates the consistent elastic-plastic modulus if the incremental equivalent plastic strain is positive.

SUBROUTINE WALKEQ - Integrates the Walker unified creep plasticity constitutive equation and also generates a material modulus based on the temperature dependent elasticity assumption.

SUBROUTINE LELAST - Calculates the stress for the constant material modulus given as data.

SUBROUTINE THRSTN - Calculates the thermal strain.

SUBROUTINE CRPSTN - Calculates the creep strain.

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